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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	May 12	EXTEND option available in structure searching
NEWS	4	May 12	Polymer links for the POLYLINK command completed in REGISTRY
NEWS	5	May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
NEWS	6	May 27	CAplus super roles and document types searchable in REGISTRY
NEWS	7	Jun 28	Additional enzyme-catalyzed reactions added to CASREACT
NEWS	8	Jun 28	ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R)
NEWS	9	Jul 12	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
NEWS	10	Jul 30	BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
NEWS	11	AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS	12	AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS	13	AUG 02	STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
NEWS	14	AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS	15	AUG 04	Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004

NEWS EXPRESS	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:54:10 ON 24 AUG 2004

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=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 14:54:19 ON 24 AUG 2004
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STRUCTURE FILE UPDATES:   23 AUG 2004  HIGHEST RN 731771-88-3
DICTIONARY FILE UPDATES:  23 AUG 2004  HIGHEST RN 731771-88-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\10771861.6

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
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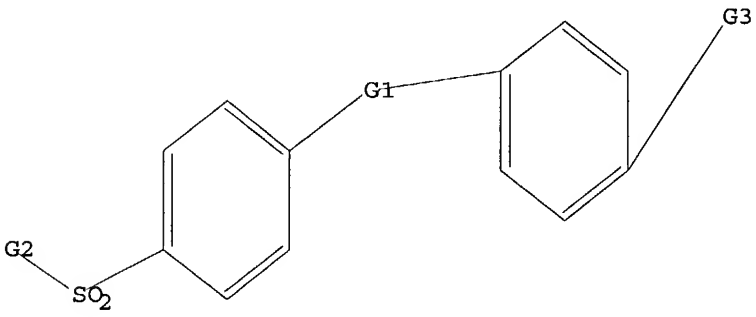

G1 Cb,Cy,Hy

G2 N,NH,NH2,Ak

G3 Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

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=> s l1 sss full
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FULL SEARCH INITIATED 14:54:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 855006 TO ITERATE

 46.8% PROCESSED  400000 ITERATIONS                              63 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.12

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:       855006 TO   855006
PROJECTED ANSWERS:             100 TO      168

L2            63 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               155.42     155.63

FILE 'CAPLUS' ENTERED AT 14:54:59 ON 24 AUG 2004
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FILE COVERS 1907 - 24 Aug 2004  VOL 141 ISS 9
FILE LAST UPDATED: 23 Aug 2004  (20040823/ED)

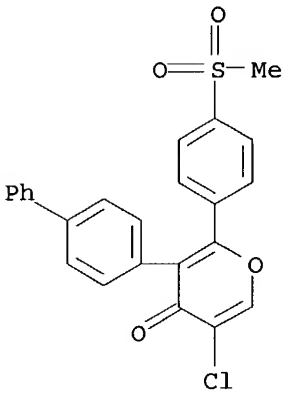
  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l2
L3            19 L2

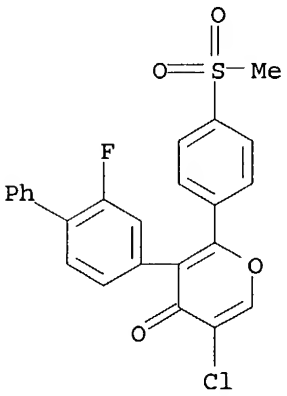
=> d l3 fbib hitstr abs total

L3   ANSWER 1 OF 19  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2004:303289  CAPLUS
DN   141:54156
TI   2,3-Diarylpyran-4-ones: a new series of selective cyclooxygenase-2
     inhibitors
AU   Joo, Yung Hyup; Kim, Jin Kwan; Kang, Seon-Hwa; Noh, Min-Soo; Ha, Jun-Yong;
     Choi, Jin Kyu; Lim, Kyung Min; Chung, Shin
CS   Pharmaceutical & Health Research Institute, Drug Discovery, AmorePacific
     Corporation R&D Center, Kyounggi-do, 449-729, S. Korea
SO   Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2195-2198
     CODEN: BMCLE8; ISSN: 0960-894X
PB   Elsevier Science B.V.
```

DT Journal
LA English
IT **708244-51-3P 708244-72-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of 2,3-diarylpyran-4-ones as cyclooxygenase-2 inhibitors and oral antiinflammatory agents)
RN 708244-51-3 CAPLUS
CN 4H-Pyran-4-one, 3-[1,1'-biphenyl]-4-yl-5-chloro-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RN 708244-72-8 CAPLUS
CN 4H-Pyran-4-one, 5-chloro-3-(2-fluoro[1,1'-biphenyl]-4-yl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



AB A new series of cyclooxygenase-2 (COX-2) inhibitors with γ-pyrone as central scaffold unit has been synthesized and their biol. activities were evaluated against cyclooxygenase inhibitory activity. The changes of phys. properties of the mols. were performed according to the medicinal chemical principles and moderate oral antiinflammatory activity was obtained with this series of inhibitors.
RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN

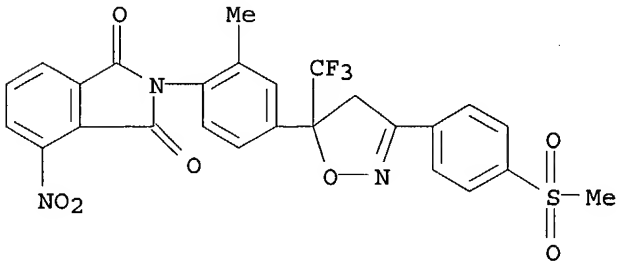
AN 2004:182828 CAPLUS
DN 140:217657
TI Preparation of N-(4-heterocyclylphenyl)phthalic acid diamide compounds as pest control agents
IN Mita, Takeshi; Kudo, Yoshihiro; Mizukoshi, Takashi; Hotta, Hiroyasu; Maeda, Kazushige; Takii, Shinji
PA Nissan Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 634 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004018410	A1	20040304	WO 2003-JP10708	20030825

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

JP 2002-244619	A	20020826
JP 2002-281294	A	20020926
JP 2002-344987	A	20021128
JP 2003-83371	A	20030325
JP 2003-182013	A	20030626

OS MARPAT 140:217657
IT **666746-24-3P**
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(4-heterocyclylphenyl)phthalic acid diamide compds. as pest control agents such as insecticides and acaricides)
RN 666746-24-3 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[4,5-dihydro-3-[4-(methylsulfonyl)phenyl]-5-(trifluoromethyl)-5-isoxazolyl]-2-methylphenyl]-4-nitro- (9CI) (CA INDEX NAME)



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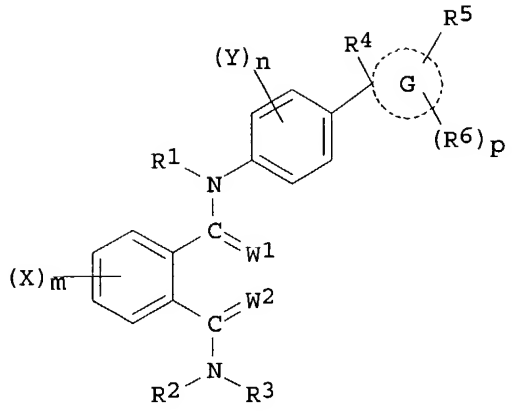


I

AB 4'-Heterocyclylbenzanilides [I; G = 5- or 6-membered nonarom. heterocyclyl containing at least one atom selected from O, S, and N and at least one double bond, 5- or 6-membered saturated heterocyclyl containing 2 atoms selected from O, S, and N, 3- to 6-membered cycloalkyl; W1, W2 = O, S; X = halo, cyano, NO2, N3, -SCN, SF5, each (un)substituted C1-6 alkyl, C3-8 cycloalkyl, C2-6 alkenyl, C2-6 alkynyl, or OH, C3-8 cycloalkenyl, C3-8 halocycloalkenyl, SH, etc.; Y = halo, cyano, NO2, N3, -SCN, SF5, each (un)substituted C1-6 alkyl, C3-8 cycloalkyl, Ph, OH, or NH2, SH, etc.; R1, R2, R3 = H, cyano, each (un)substituted C1-12 alkyl, C3-12 cycloalkyl, C3-12 alkenyl, C3-12 alkynyl, PhO, phenyl-C1-4 alkoxy, PhS, or Ph, C3-12 cycloalkenyl, C3-12 halocycloalkenyl, C1-6 alkylthio, C1-6 haloalkylthio, etc.; R4 = H, halo, cyano, each (un)substituted C1-6 alkyl, C1-6 haloalkyl, C3-8 cycloalkyl, Ph, or OH, C3-6 alkenyl, C3-6 haloalkenyl, C3-6 alkynyl, C3-6 haloalkyl, 1-naphthyl, 2-naphthyl, etc.; R5 = H, halo, cyano, each (un)substituted C1-6 alkyl, C1-6 haloalkyl, C3-8 cycloalkyl, C3-8 halocycloalkyl, or OH, C3-6 alkenyl, C3-6 haloalkenyl, C3-6 alkynyl, C3-6 haloalkynyl, etc.; R6 = H, halo, cyano, each (un)substituted C1-6 alkyl, C1-6 haloalkyl, C3-8 cycloalkyl, C3-8 halocycloalkyl, or Ph, C1-6 alkoxy, C1-6 haloalkoxy, 1-naphthyl, 2-naphthyl, etc.; m, n = an integer of 0-4; p = an integer of 0-9] or salts thereof. Also disclosed is a novel agricultural chemical, especially an insecticide or acaricide containing the compound I as the active ingredient. For example, N1-[4-[3-(4-fluorophenyl)-5-trifluoromethyl-4,5-dihydroisoxazol-5-yl]-2-methylphenyl]-3-nitro-N2-isopropylphthaldiamide and N1-[4-[6-(4-chlorophenyl)-2-methyl-4-trifluoromethyl-3,4-dihydropyrimidin-4-yl]-2-methylphenyl]-3-iodo-N2-isopropylphthaldiamide at 100 ppm controlled ≥80% 2nd instar larvae of Spodoptera litura on cabbage leaves.

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:836766 CAPLUS
DN 139:350731
TI Preparation of 1-phenyl-1H-pyrazoles for inducing apoptosis in proliferating cells
IN Chen, Ching-shin; Song, Xueqin; Lin, Ho-pi
PA The Ohio State University Research Foundation, USA

SO PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

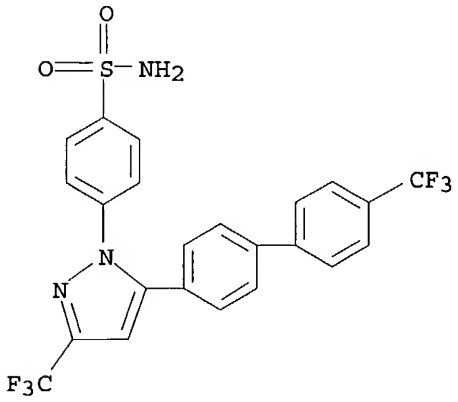
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003086287	A2	20031023	WO 2003-US10738	20030408
WO 2003086287	A3	20040325		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

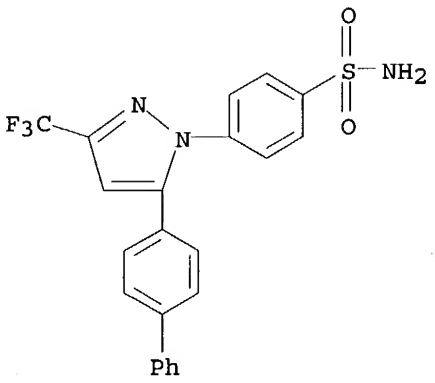
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

			US 2002-370664P	P 20020408
US 2003236294	A1	20031225	US 2003-409502	20030408
			US 2002-370664P	P 20020408

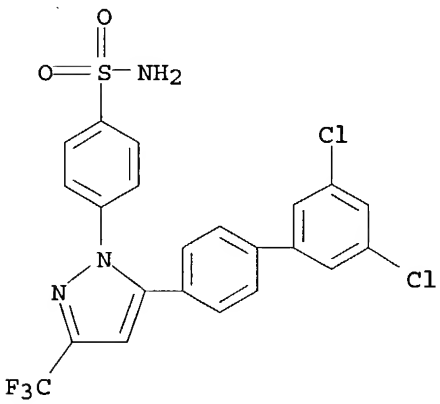
OS MARPAT 139:350731
IT **618068-95-4P 618068-99-8P 618069-00-4P**
618069-08-2P 618069-09-3P 618069-10-6P
618069-11-7P 618069-12-8P 618069-13-9P
618069-14-0P 618069-15-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiproliferative agent; preparation of 1-Ph-1H-pyrazoles for inducing apoptosis in proliferating cells)
RN 618068-95-4 CAPLUS
CN Benzenesulfonamide, 4-[3-(trifluoromethyl)-5-[4'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



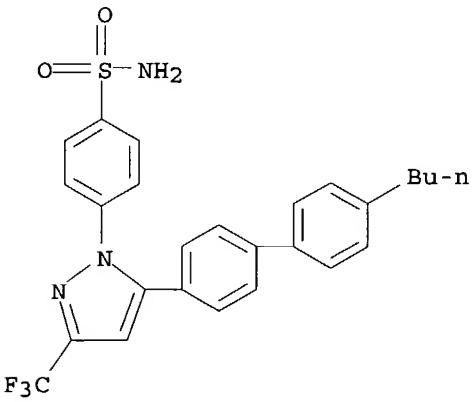
RN 618068-99-8 CAPLUS
CN Benzenesulfonamide, 4-[5-[1,1'-biphenyl]-4-yl-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



RN 618069-00-4 CAPLUS
CN Benzenesulfonamide, 4-[5-(3',5'-dichloro[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

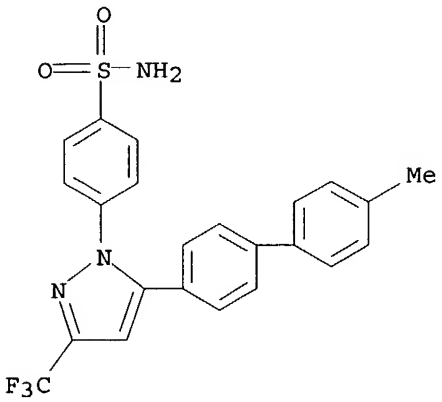


RN 618069-08-2 CAPLUS
CN Benzenesulfonamide, 4-[5-(4'-butyl[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

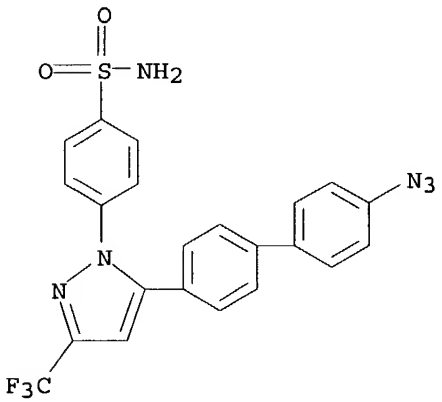


RN 618069-09-3 CAPLUS

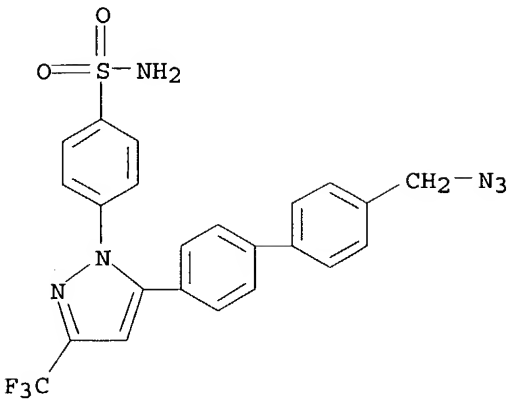
CN Benzenesulfonamide, 4-[5-(4'-methyl[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



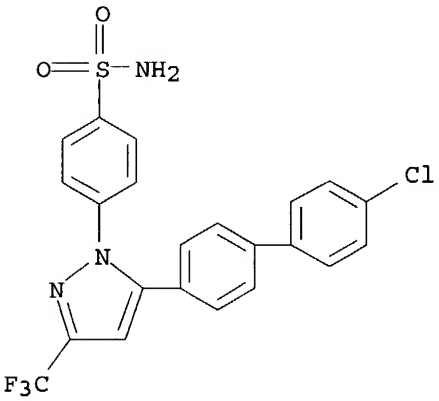
RN 618069-10-6 CAPLUS
CN Benzenesulfonamide, 4-[5-(4'-azido[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



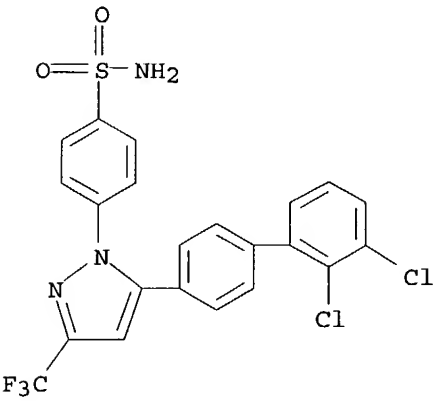
RN 618069-11-7 CAPLUS
CN Benzenesulfonamide, 4-[5-[4'-(azidomethyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



RN 618069-12-8 CAPLUS
CN Benzenesulfonamide, 4-[5-(4'-chloro[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

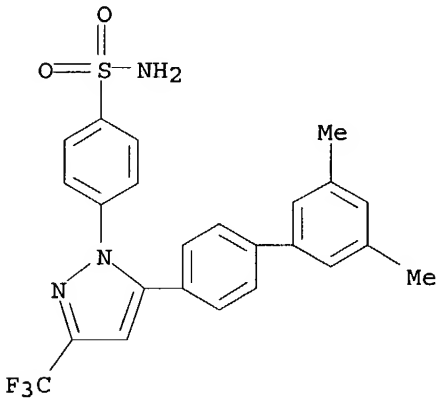


RN 618069-13-9 CAPLUS
CN Benzenesulfonamide, 4-[5-(2',3'-dichloro[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

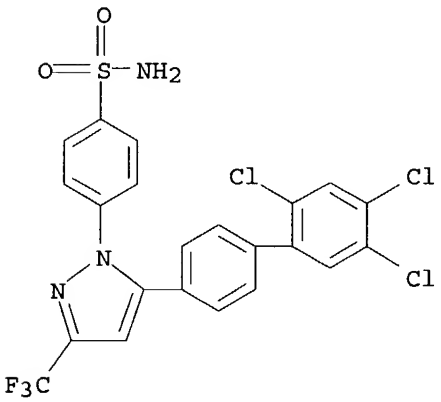


RN 618069-14-0 CAPLUS

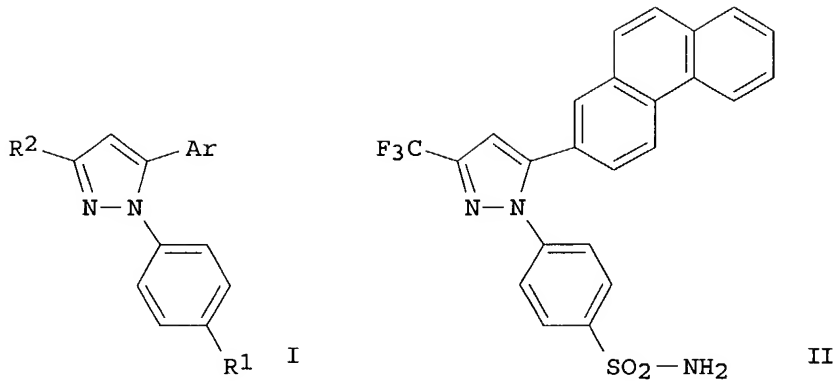
CN Benzenesulfonamide, 4-[5-(3',5'-dimethyl[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



RN 618069-15-1 CAPLUS
CN Benzenesulfonamide, 4-[5-(2',4',5'-trichloro[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



GI



I II

AB Title compds. I [wherein R1 = carboxamido; R2 = (halo)alkyl; Ar = (un)substituted Ph biphenyl, naphthyl, anthryl, phenanthrenyl, or fluorenyl; and pharmaceutically acceptable salts thereof] were prepared and tested for their effects on cyclooxygenase-2 (COX-2) activity, the viability of human prostate cancer PC-3 cells, and their ability to induce apoptosis in these cells. For example, Claisen condensation of 2-acetylphenanthrene with Et trifluoroacetate in the presence of NaH afforded the 1,3-keto-enol derivative (95%). Reaction with (4-sulfamoylphenyl)hydrazine•HCl in EtOH gave 4-[5-(2-phenanthrenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (II) in 65% yield. A structure-activity anal. of derivs. of the COX-2 inhibitor celecoxib found no correlation between the COX-2 inhibitory and apoptosis-inducing activities. For instance, increased polarity or bulkiness of the terminal Ph ring reduced the ability of compds. to inhibit COX-2, while a certain degree of bulkiness and hydrophobicity in the substituted Ph ring was highly desirable for apoptosis induction in PC-3 cells. Thus, I are useful for inducing apoptosis in proliferating cells, particularly cancer cells, including but not limited to prostate cancer, leukemia, non-small cell lung cancer, colon cancer, CNS cancer, melanoma, ovarian cancer, renal cancer, bladder cancer, lymphoma, and breast cancer. These compds. are particularly useful in the treatment of androgen-independent cancers, including hormone-refractory prostate cancer.

L3 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:777577 CAPLUS
DN 139:286336
TI Medicinal composition containing inhibitor of decomposition of extracellular matrix of cartilage
IN Gemba, Takefumi; Okamoto, Hiroyuki; Watanabe, Fumihiko
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 101 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003080042	A1	20031002	WO 2003-JP3673	20030326

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH,

PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,
RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
GW, ML, MR, NE, SN, TD, TG

JP 2002-87330 A 20020327

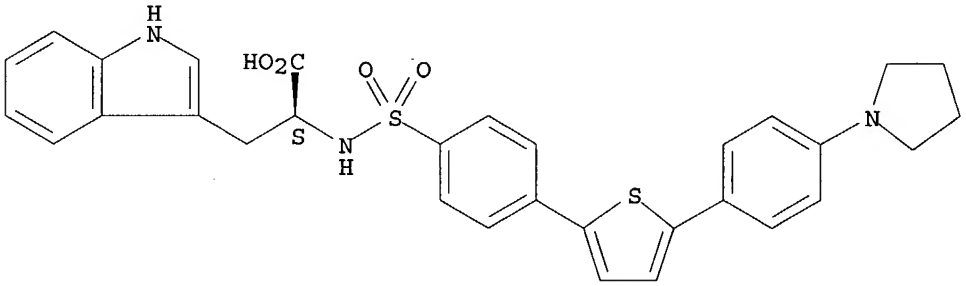
OS MARPAT 139:286336

IT **607719-52-8P 607719-58-4P 607719-60-8P**
607719-61-9P 607719-62-0P 607719-63-1P
607719-64-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(medicinal composition containing inhibitor of decomposition of extracellular matrix
of cartilage and preparation of said inhibitor)

RN 607719-52-8 CAPLUS

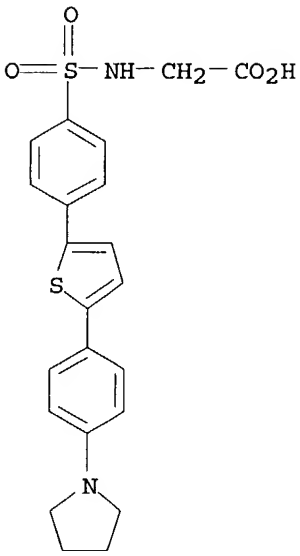
CN L-Tryptophan, N-[[4-[5-[4-(1-pyrrolidinyl)phenyl]-2-thienyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



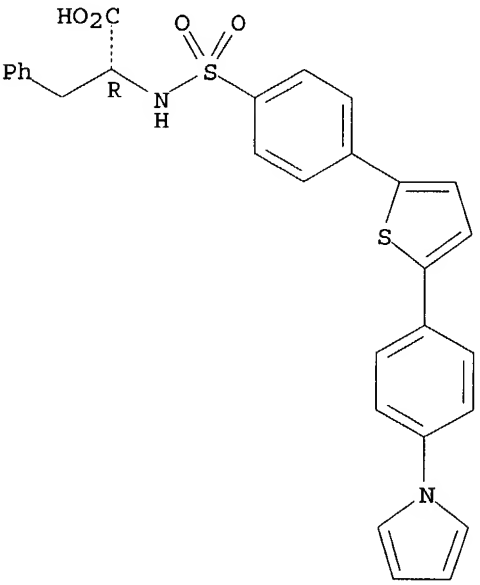
RN 607719-58-4 CAPLUS

CN Glycine, N-[[4-[5-[4-(1-pyrrolidinyl)phenyl]-2-thienyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



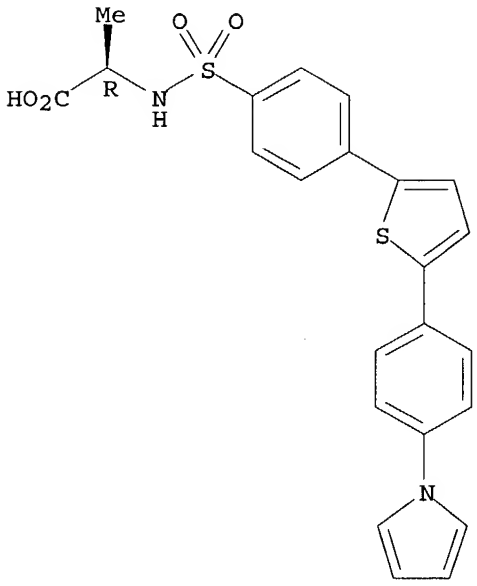
RN 607719-60-8 CAPLUS
CN D-Phenylalanine, N-[[4-[5-[4-(1H-pyrrol-1-yl)phenyl]-2-thienyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



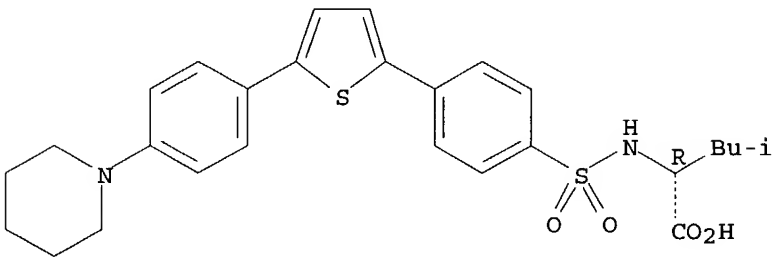
RN 607719-61-9 CAPLUS
CN D-Alanine, N-[[4-[5-[4-(1H-pyrrol-1-yl)phenyl]-2-thienyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



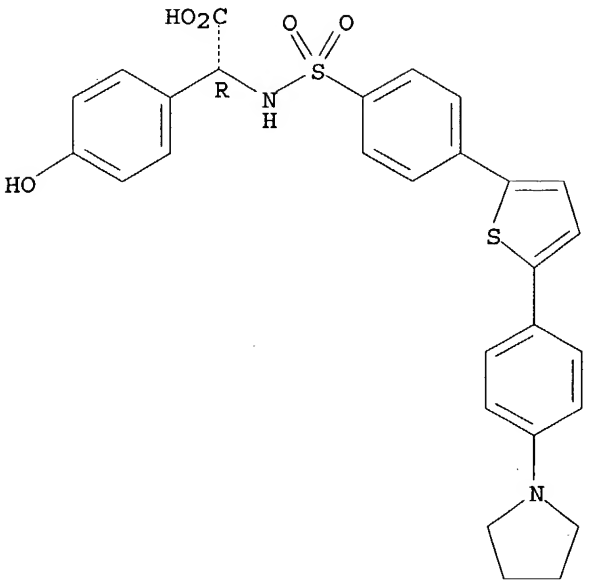
RN 607719-62-0 CAPLUS
CN D-Leucine, N-[[4-[5-[4-(1-piperidinyl)phenyl]-2-thienyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



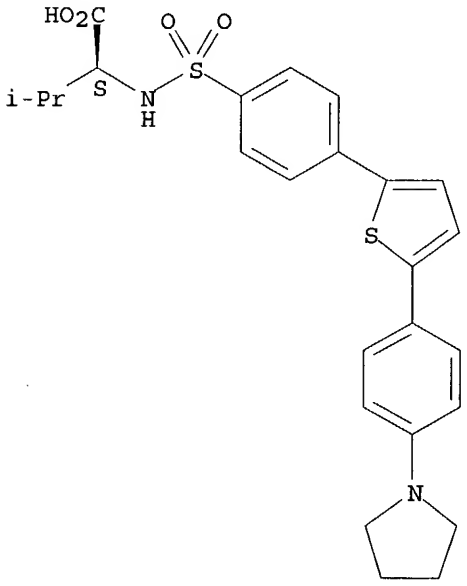
RN 607719-63-1 CAPLUS
CN Benzeneacetic acid, 4-hydroxy-α-[[[4-[5-[4-(1-pyrrolidinyl)phenyl]-2-thienyl]phenyl]sulfonyl]amino]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 607719-64-2 CAPLUS
CN L-Valine, N-[[4-[5-[4-(1-pyrrolidinyl)phenyl]-2-thienyl]phenyl]sulfonyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB A medicinal composition contains a compound represented by the general formula R6R5R4SO2W [W is R3NCH(R2)COR1, etc.; R1 is hydroxy, etc.; R2 is optionally substituted lower alkyl, etc.; R3 is hydrogen, etc.; R4 is optionally substituted arylene, etc.; R5 is a single bond, CO, etc.; and R6 is optionally substituted aryl, etc.], an optically active isomer thereof, a prodrug thereof, a pharmaceutically acceptable salt of any of these, or a solvate of any of these. Compds. of this invention in vitro

showed IC50 values of 0.00045 μM to >10 μM against MMP-13. Formulations are given.

RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:221693 CAPLUS
DN 138:238197
TI Preparation of furo- and thienopyrimidines as TIE-2 and/or VEGFR-2 kinase inhibitors useful against hyperproliferative diseases
IN Adams, Jerry Leroy; Bryan, Deborah Lynne; Feng, Yanhong; Matsunaga, Shinichiro; Maeda, Yutaka; Miyazaki, Yasushi; Nakano, Masato; Rocher, Jean-Philippe; Sato, Hideyuki; Semones, Marcus; Silva, Domingos J.; Tang, Jun
PA Glaxosmithkline K.K., Japan; Smithkline Beecham Corporation
SO PCT Int. Appl., 265 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003022852	A2	20030320	WO 2002-US28650	20020910
WO 2003022852	A3	20031127		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

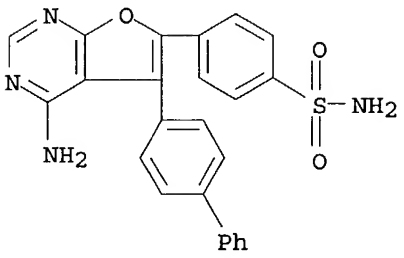
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

			US 2001-318766P	P 20010911
EP 1425284	A2	20040609	EP 2002-798181	20020910

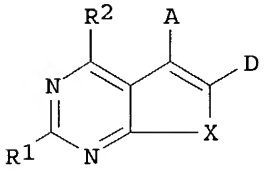
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, SK

US 2001-318766P	P	20010911
WO 2002-US28650	W	20020910

OS MARPAT 138:238197
IT **501695-52-9P**, 4-Amino-5-(4-biphenylyl)-6-(4-sulfamoylphenyl)furo[2,3-d]pyrimidine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of furo- and thienopyrimidines as TIE-2 and/or VEGFR-2 kinase inhibitors useful against hyperproliferative diseases)
RN 501695-52-9 CAPLUS
CN Benzenesulfonamide, 4-(4-amino-5-[1,1'-biphenyl]-4-ylfuro[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)



GI



I

AB Furo- and thienopyrimidine derivs. (shown as I; variables defined below; e.g. 4-Amino-3-(4-methoxyphenyl)-2-[3-(methylsulfonylamino)phenyl]furo[2,3-d]pyrimidine), which are useful as TIE-2 (tyrosine kinase containing immunoglobin and EGF homol. domains) and/or VEGFR-2 kinase inhibitors against hyperproliferative diseases are described herein. Enzyme inhibitions by .apprx.60 examples of I are included as ranges; also, 4-amino-3-[4-[[2-fluoro-5-(trifluoromethyl)phenyl]aminocarbonylamino]phenyl]thieno[2,3-d]pyrimidine exhibited IC50 = 0.0018 μM in the TIE-2 fluorescence polarization kinase activity assay. For I: X is O or S; A is H, halo, C1-C6 alkyl, aryl, heteroaryl, aryl or heteroaryl substituted with ≥1 R3, heterocyclyl, -RR3, -C(O)OR4, -C(O)NR5R6, -C(O)R4; D is H, halo, C1-C6 alkyl, aryl, heteroaryl, aryl or heteroaryl substituted with ≥1 R3, heterocyclyl, -RR3, -C(O)OR4, -C(O)NR5R6, or -C(O)R4. R is C1-C6 alkylene, C3-C7 cycloalkylene, C1-C6 alkenylene, or C1-C6 alkynylene; R1 is H, C1-C6 alkyl, C1-C6 alkoxy, -SR4, -S(O)2R4, -NR7R7, -NR'N R'''R'''', -N(H)RR3, -C(O)OR7, or -C(O)NR7R7. R2 is H, -OH, -NR7R7 or :NH; R3 is halo, C1-C6 alkyl, C1-C6 haloalkyl, C1-C6 alkoxy, C3-C7 cycloalkoxy, C1-C6 haloalkoxy, aryl, aralkyl, aryloxy, heteroaryl, heterocyclyl, -CN, -NHC(O)R4, -N(R8)HC(O)R4, -NHC(S)R4, -NR5R6, -RNR5R6, -SR4, -S(O)2R4, -RC(O)OR4, -C(O)OR4, -C(O)R4, -C(O)NR5R6, -NHS(O)2R4, -N(S(O)2R4)S(O)2R4, -S(O)2NR5R6, or -NHC(:NH)R4. R4 is H, C1-C6 alkyl, aryl, heteroaryl, heterocyclyl, -RR3, -NR'''R'''', or - NR'NR'''R''''; R5 is H, C1-C6 alkyl, C3-C7 cycloalkyl, cyanoalkyl, -R'R'', aryl, aralkyl, heteroaryl, -NHC(O)OR''', -R'NHC(O)OR''', -R'NHC(O)NR'''R'''', or -R'C(O)OR'''. R6 is H, C1-C6 alkyl, C3-C7 cycloalkyl, cyanoalkyl, -R'R'', aryl, aralkyl, heteroaryl, -C(O)OR''', or -R'C(O)NR'''R'''; R7 is H, C1-C6 alkyl, aryl, or -C(O)OR'''; R8 is C1-C3 alkyl; R' is C1-C3 alkylene; R'' is heteroalkyl or NRR'''R''''; R''' is H, C1-C6 alkyl, aryl, aralkyl, heteroaryl, or C3-C7 cycloalkyl; R'''' is H, C1-C6 alkyl, aryl, heteroaryl, or C3-C7 cycloalkyl. Although the methods of preparation are not claimed, several example prepns. of I are included and characterization data is given for .apprx.480 examples of I.

L3 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:69769 CAPLUS
DN 138:364359

TI Voltage-dependent formation of anion channels by synthetic rigid-rod push - pull β-barrels

AU Sakai, Naomi; Houdebert, David; Matile, Stefan
CS Department of Organic Chemistry, University of Geneva, Geneva, 1211/4, Switz.

SO Chemistry--A European Journal (2003), 9(1), 223-232
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English

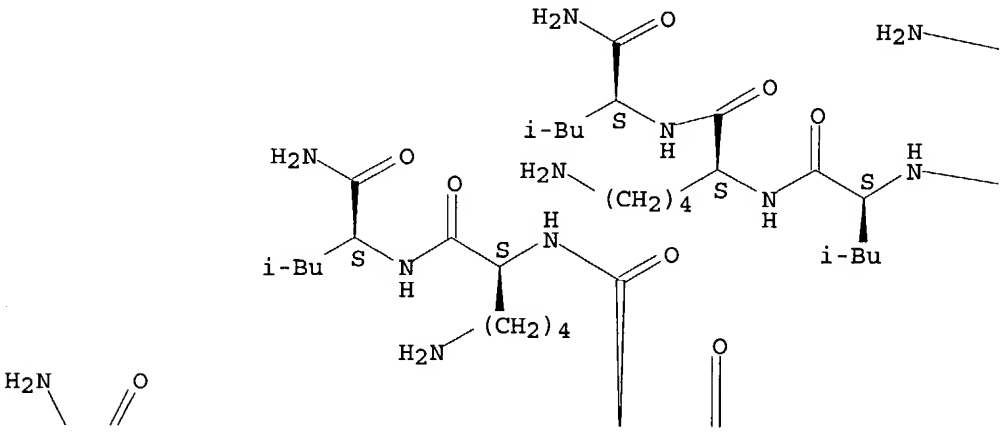
IT **406217-64-9**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(voltage-dependent formation of anion channels by synthetic rigid-rod push-pull β-barrels)

RN 406217-64-9 CAPLUS

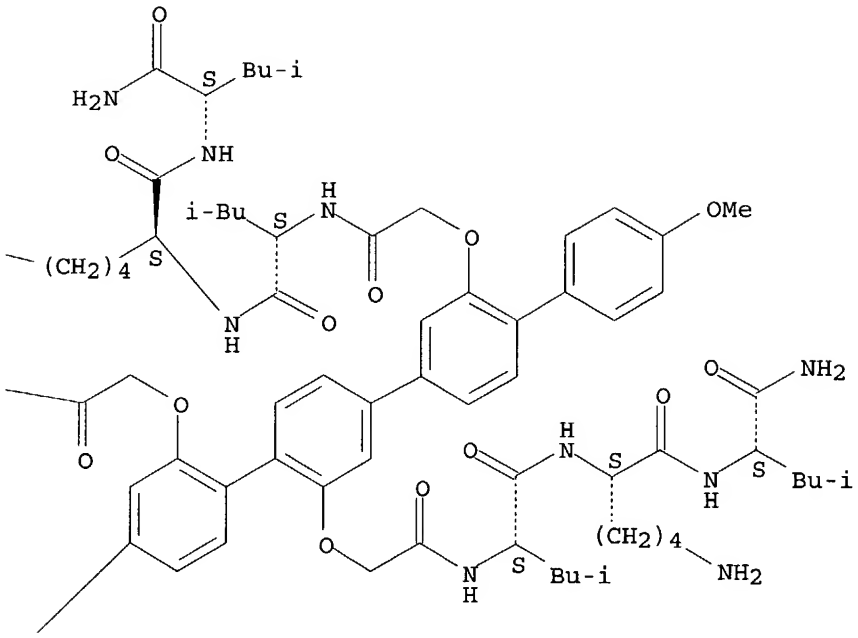
CN L-Leucinamide, 1,1',1'',1''',1'''',1''''',1'''''-[[4-methoxy-4'''''''-(methylsulfonyl)[1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1'''''':4'''''',1''''''':4'''''''-octiphenyl]-2',2''',2''''',3'',3'''',3''''''-hexayl]hexakis[oxy(1-oxo-2,1-ethanediyl)]]hexakis[L-leucyl-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

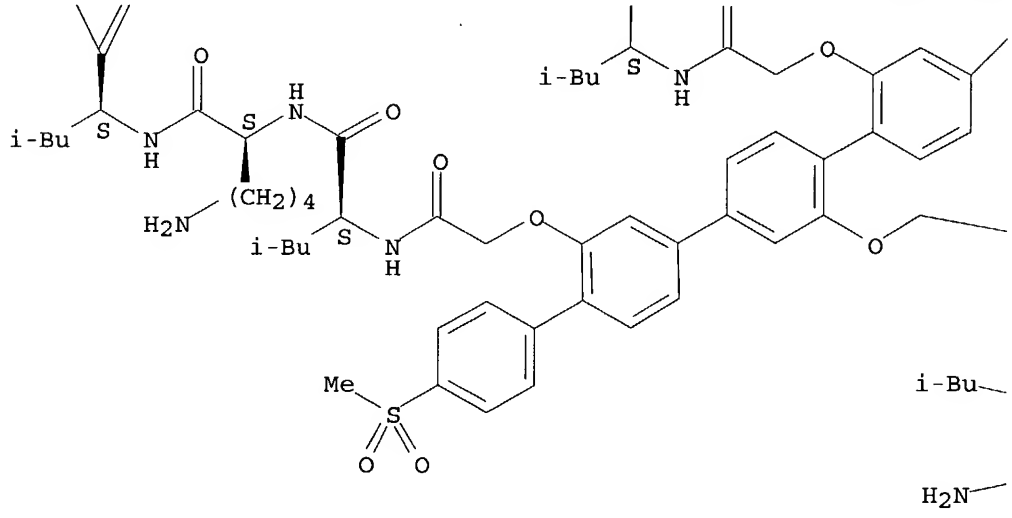
PAGE 1-A



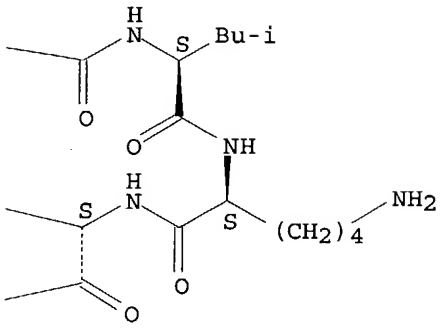
PAGE 1-B



PAGE 2-A



PAGE 2-B



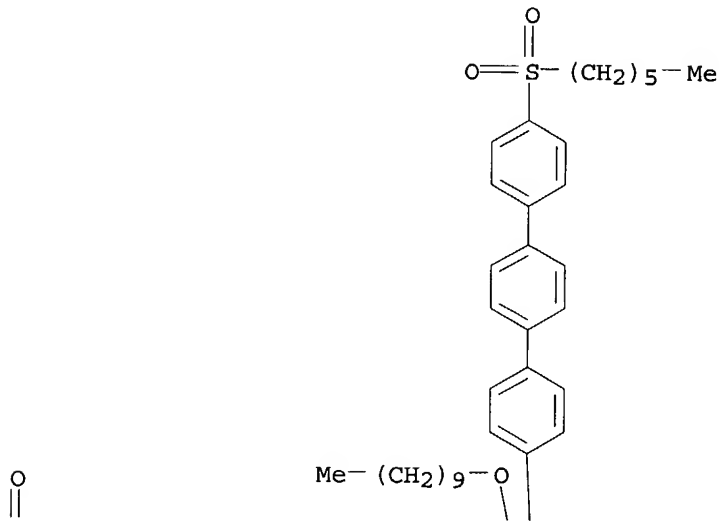
AB Ion channels formed by p-octiphenyls equipped with amphiphilic, cationic tripeptide strands and either with (5) or without (6) axial dipole moment are described (preliminary communication: N. Sakai, S. Matile, J. Am. Chemical Society 2002, 124, 1184-1185). Fluorescence kinetics with variably polarized neutral or anionic vesicles, together with planar bilayer conductance measurements, reveal voltage dependence with weakly lyotropic anion selectivity, and deactivation by competing surface potentials of the ion channels formed by asym. 5. In planar bilayers, 5 forms short-lived, poorly organized channels-similar to those produced by α-helical natural antibiotics-capable of transforming into stable, ohmic p-octiphenyl "β-barrel" ion channels similar to those of the >99% homologous but sym. 6. Fluorescence depth quenching and CD studies confirm the effect of membrane potentials in promotion of the partitioning of 5 (but not 6) into the bilayers, identifying partitioning as the voltage-dependent step.

RE.CNT 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:22325 CAPLUS
DN 139:6667
TI Synthesis and fluorescence enhancement of oligophenylene-substituted calix[4]arene assemblies
AU Wong, Man Shing; Zhang, Xiao Ling; Chen, Dong Zhong; Cheung, Wai Ho
CS Department of Chemistry, Hong Kong Baptist University, Hong Kong, Peop. Rep. China
SO Chemical Communications (Cambridge, United Kingdom) (2003), (1), 138-139
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 139:6667
IT **536708-84-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of oligophenylene-substituted calixarene assemblies via cross-coupling reaction of oligoboronic acid and tetrahalocalixarenes and their fluorescence enhancement)
RN 536708-84-6 CAPLUS

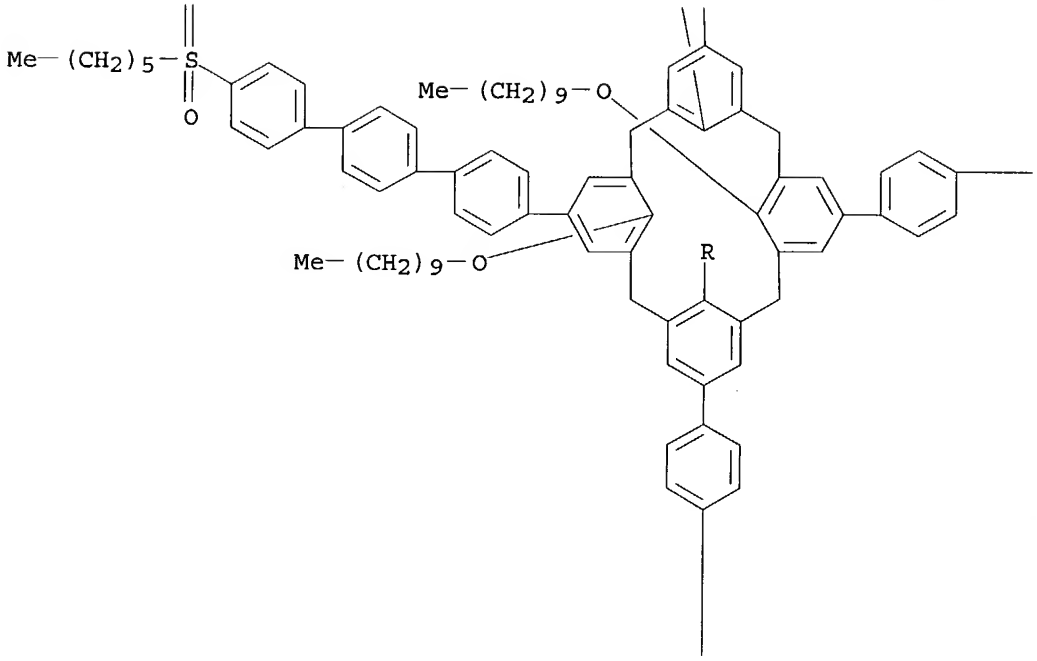
CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene, 25,26,27,28-tetrakis(decyloxy)-5,11,17,23-tetrakis[4''-(hexylsulfonyl)[1,1':4',1''-terphenyl]-4-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

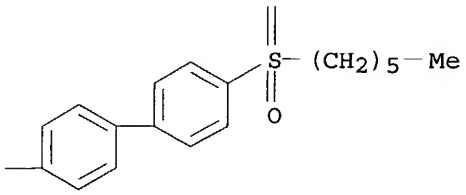


PAGE 1-B

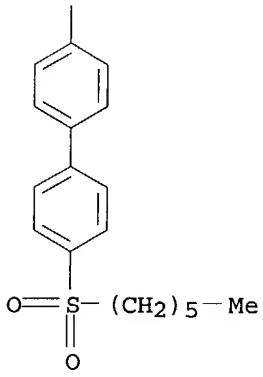
PAGE 2-A

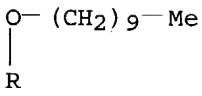


PAGE 2-B



PAGE 3-A





AB Tetra-oligophenylene substituted calix[4]arene assemblies containing up to three phenylene units have been synthesized by a convergent approach using Suzuki cross-coupling reaction. Their optical properties were investigated and compared with the corresponding monomer.

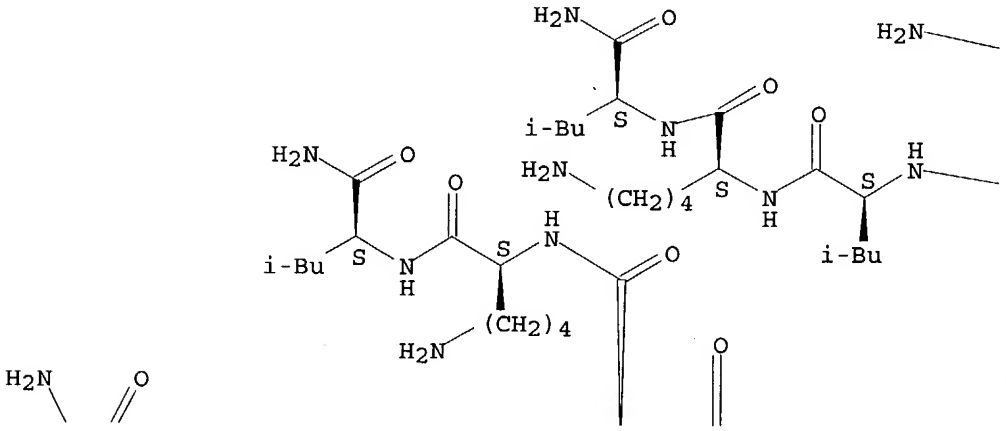
RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:805629 CAPLUS
DN 138:200393
TI On the importance of intermediate internal charge repulsion for the synthesis of multifunctional pores
AU Baumeister, Bodo; Som, Abhigyan; Das, Gopal; Sakai, Naomi; Vilbois, Francis; Gerard, David; Shahi, Shatrughan P.; Matile, Stefan
CS Department of Organic Chemistry, University of Geneva, Geneva, CH-1211/4, Switz.
SO Helvetica Chimica Acta (2002), 85(9), 2740-2753
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
OS CASREACT 138:200393
IT **406217-64-9**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(importance of intermediate internal charge repulsion for synthesis of

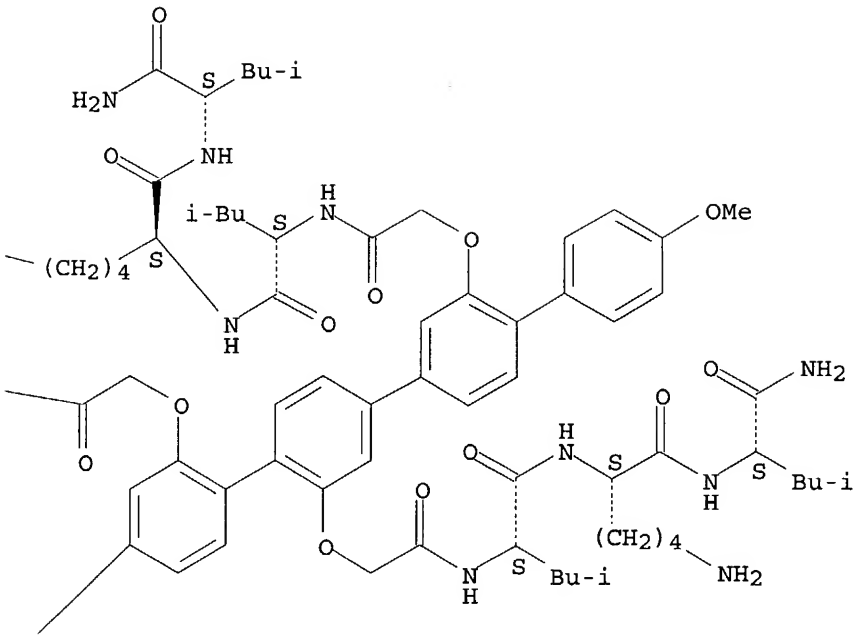
multifunctional pores)
RN 406217-64-9 CAPLUS
CN L-Leucinamide, 1,1',1'',1''',1'''',1''''',1'''''-[[4-methoxy-4'''''''-(methylsulfonyl)[1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1'''''':4'''''',1''''''':4'''''''-octiphenyl]-2',2''',2''''',3'',3'''',3''''''-hexayl]hexakis[oxy(1-oxo-2,1-ethanediyl)]]hexakis[L-leucyl-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

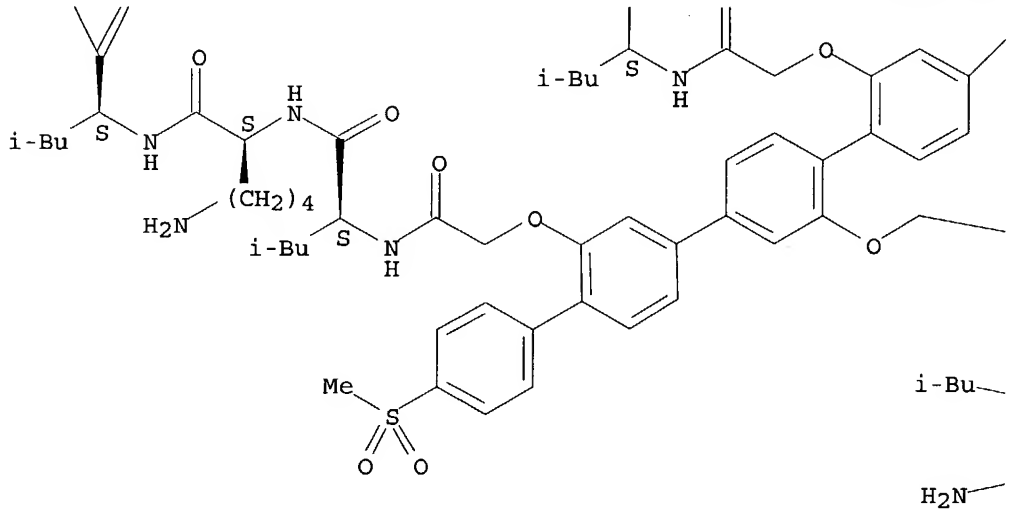
PAGE 1-A

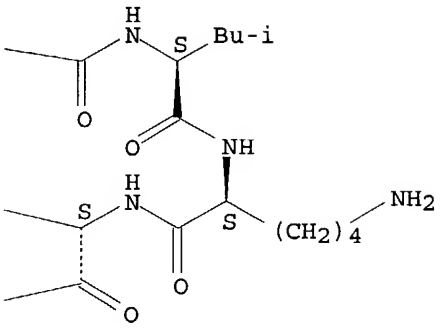


PAGE 1-B



PAGE 2-A





AB Intermediate internal charge repulsion (ICR) is required to create synthetic pores with large, stable, transmembrane, and variably functionalized space. This conclusion is drawn from maximal transport and, in one case, catalytic activity of p-octiphenyl β-barrel pores with internal lysine, aspartate, and histidine residues around pH 7, 6, and 4.5, resp. PKa Simulations corroborate the exptl. correlation of intermediate ICR with activity and suggest that insufficient ICR causes pore "implosion" and excess ICR pore "explosion". Esterolysis expts. support the view that the formation of stable space within multifunctional p-octiphenyl β-barrels requires more ICR in bilayer membranes than in H2O. Multivalency effects are thought to account for p-octiphenyl β-barrel expansion with increasing number of β-sheets, and proximity effects for unchanged pH profiles with increasing β-sheet length. Q-TOF-nano-ESI-MS barrel-denaturation expts. indicate that contributions from internal counterion effects are not negligible. The overall characteristics of p-octiphenyl β-barrel pores with internal lysine, aspartate, and histidine residues, unlike de novo "α-barrels" and similarly to certain biol. channels, underscore the usefulness of rigid-rod mols. to preorganize complex multifunctional supramol. architecture.

RE.CNT 102 THERE ARE 102 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:793608 CAPLUS
DN 137:310917
TI Aromatic-substituted thiohydantoins, their preparation, and their use for treating diabetes, dyslipidemia, and obesity
IN Boubia, Benaiessa; Chaput, Evelyne; Ou, Khan; Ratel, Philippe
PA Laboratoires Fournier SA, Fr.
SO PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002081453	A1	20021017	WO 2002-FR1167	20020404

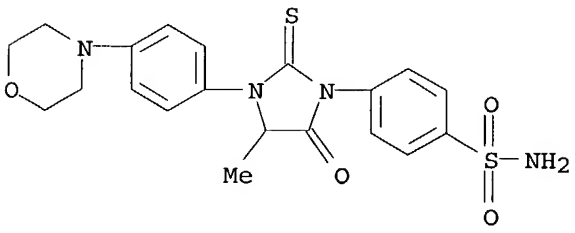
WO 2002081453		C1	20021114		
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
				FR 2001-4552	A 20010404
FR 2823209		A1	20021011	FR 2001-4552	20010404
FR 2823209		B1	20031212		
EP 1373219		A1	20040102	EP 2002-730333	20020404
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
				FR 2001-4552	A 20010404
				WO 2002-FR1167	W 20020404
EE 200300485		A	20040216	EE 2003-485	20020404
				FR 2001-4552	A 20010404
				WO 2002-FR1167	W 20020404
JP 2004525175		T2	20040819	JP 2002-579441	20020404
				FR 2001-4552	A 20010404
				WO 2002-FR1167	W 20020404
US 2004116417		A1	20040617	US 2003-473032	20030926
				FR 2001-4552	A 20010404
				WO 2002-FR1167	W 20020404
NO 2003004430		A	20031006	NO 2003-4430	20031003
				FR 2001-4552	A 20010404
				WO 2002-FR1167	W 20020404

OS MARPAT 137:310917

IT **471937-21-0P**, 1-(4-(Morpholin-4-yl)phenyl)-3-(4-(aminosulfonyl)phenyl)-5-methyl-2-thioxo-4-imidazolidinone
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aromatic-substituted thiohydantoins for treatment of diabetes, dyslipidemia, and obesity)

RN 471937-21-0 CAPLUS

CN Benzenesulfonamide, 4-[4-methyl-3-[4-(4-morpholinyl)phenyl]-5-oxo-2-thioxo-1-imidazolidinyl]- (9CI) (CA INDEX NAME)



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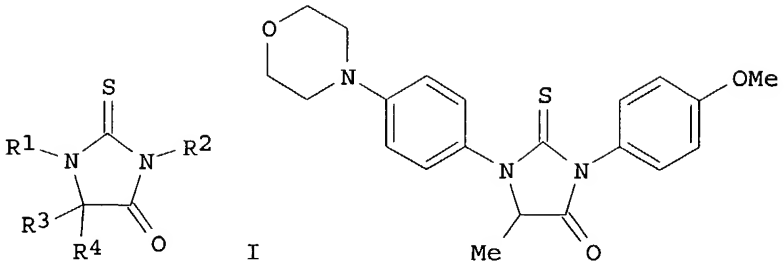


I II

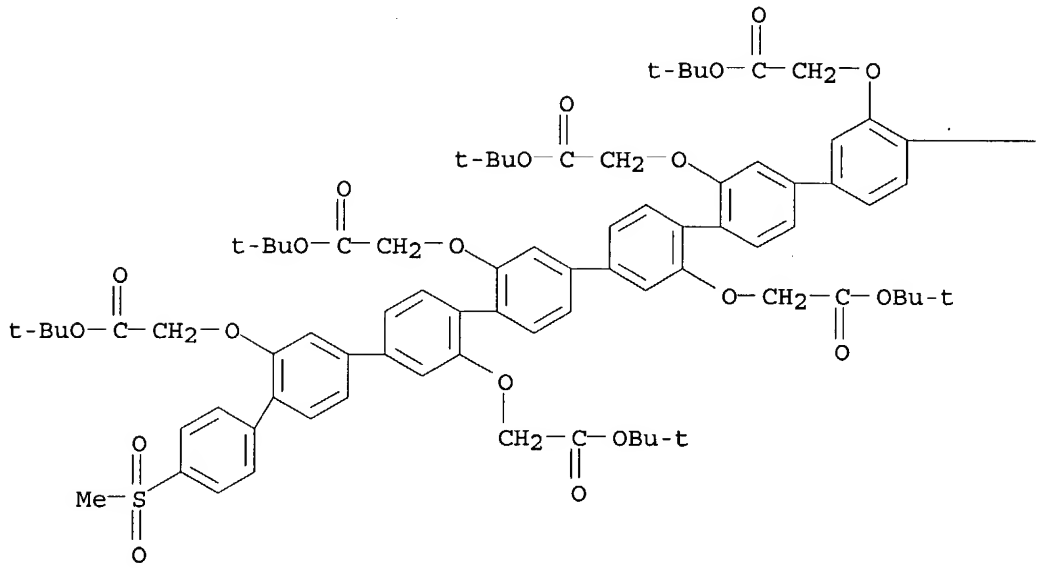
AB The invention concerns compds. derived from 2-thiohydantoin, selected among compds. I [R1 = (un)substituted aromatic nucleus [substituents = halo, alkoxy, alkyl, alkylthio, NO2, CF3, OCF3, OCH2O, or (un)substituted (homo)(thio)morpholine, (homo)piperidine, (homo)piperazine, etc.]; R2 = H, alkyl or cycloalkyl [optionally interrupted by O atoms(s)], haloalkyl, alkenyl, alkynyl, hydroxyalkyl, aminoalkyl, cyanoalkyl, (un)substituted aromatic nucleus; R3 = H, alkyl; R4 = H, alkyl, OH; or R3R4 = CH2; provided that at least one of R1 and R2 is an aromatic nucleus bearing at least one (un)substituted (homo)(thio)morpholine, (homo)piperidine, (homo)piperazine, etc.] and their addition salts with acids, in particular their pharmaceutically acceptable salts. The invention also concerns methods for preparing I, pharmaceutical compns. containing them, and their use as pharmacol. active substances, in particular for treating diabetes, diseases mediated by hyperglycemia, hypertriglyceridemia, dyslipidemia, or obesity. A total of 380 invention compds. and approx. 80 intermediates were prepared and characterized. When tested orally in mice at doses below 200 mg/kg, I reduced glucose levels by up to -73%, and reduced serum triglycerides by up to -56%, with favorable changes in lipid parameters (no specific data). For instance,4-(4-morpholinyl)aniline reacted with Et 2-bromopropionate and NaOAc in EtOH to give 69% N-[4-(4-morpholinyl)phenyl]-DL-alanine Et ester. Cyclocondensation of this amino ester with 4-(isothiocyanato)anisole in refluxing toluene in the presence of AcOH gave 82.5% title compound II.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

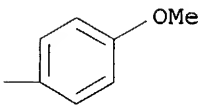
L3 ANSWER 10 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:73773 CAPLUS
DN 136:275111
TI Recognition of Polarized Lipid Bilayers by p-Oligophenyl Ion Channels: From Push-Pull Rods to Push-Pull Barrels
AU Sakai, Naomi; Matile, Stefan
CS Department of Organic Chemistry, University of Geneva, Geneva, CH-1211, Switz.
SO Journal of the American Chemical Society (2002), 124(7), 1184-1185
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
IT **406217-67-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of p-oligophenyl push-pull β-barrel synthetic ion channels which recognize phosphatidylcholine bilayer membranes)

RN 406217-67-2 CAPLUS
CN Acetic acid, 2,2',2'',2''',2'''',2'''''-[[4-methoxy-4'''''''-(methylsulfonyl)[1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1'''''':4'''''',1''''''':4'''''''-octiphenyl]-2',2''',2''''',3'',3'''',3''''''-hexayl]hexakis(oxy)]hexakis-, hexakis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A



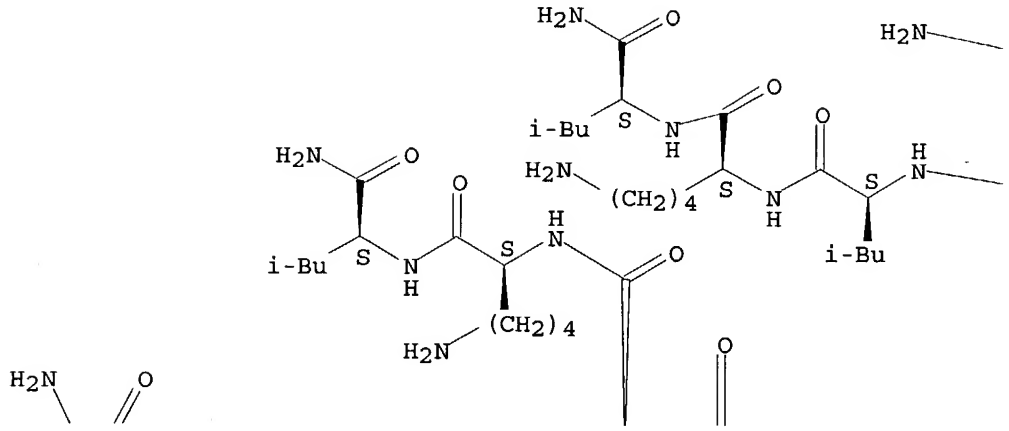
PAGE 1-B



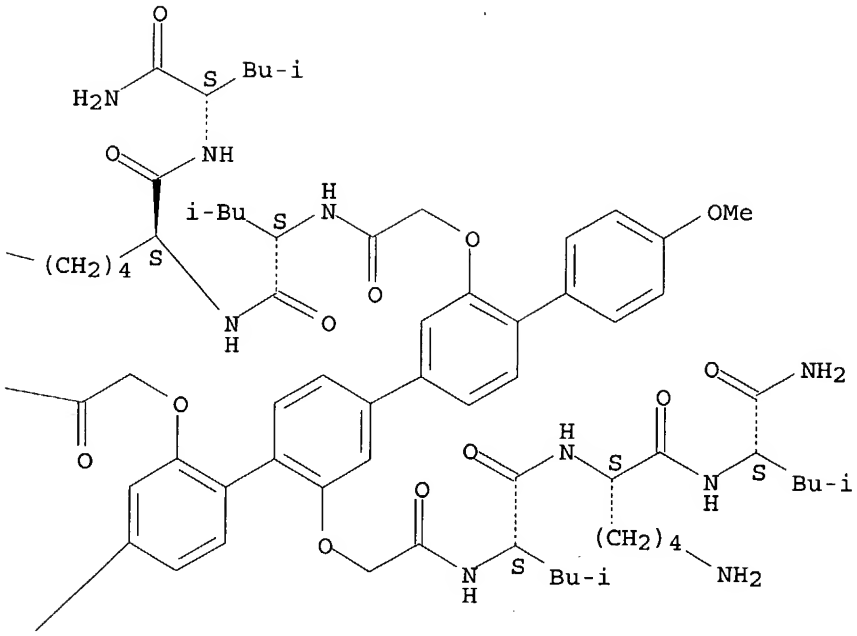
IT **406217-64-9P**
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of p-oligophenyl push-pull β-barrel synthetic ion channels which recognize phosphatidylcholine bilayer membranes)
RN 406217-64-9 CAPLUS
CN L-Leucinamide, 1,1',1'',1''',1'''',1'''''-[[4-methoxy-4'''''''-(methylsulfonyl)[1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1'''''':4'''''',1''''''':4'''''''-octiphenyl]-2',2''',2''''',3'',3'''',3''''''-hexayl]hexakis[oxy(1-oxo-2,1-ethanediyl)]]hexakis[L-leucyl-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

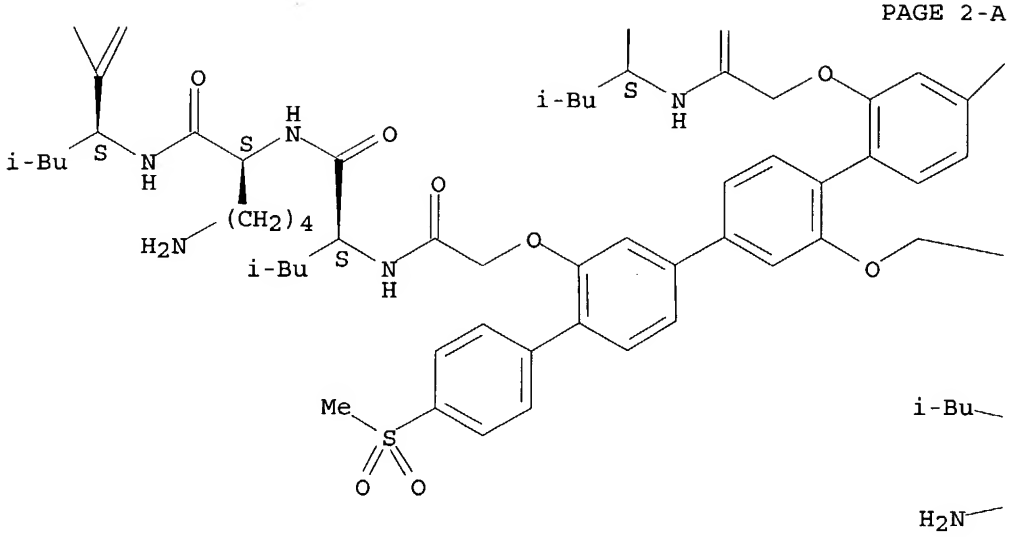
PAGE 1-A



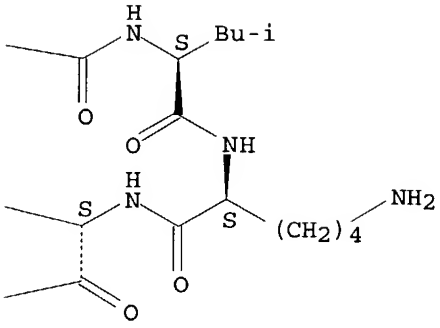
PAGE 1-B



PAGE 2-A



PAGE 2-B



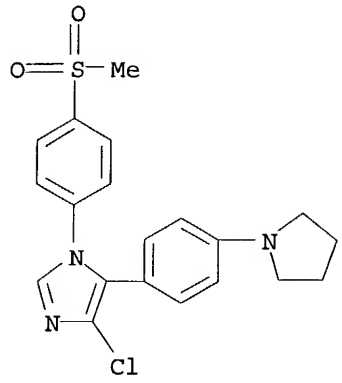
AB Design, synthesis, and evaluation of 14-methoxy-84-methylsulfonyl-22,33,42,53,62,73-hexa(Gla-Leu-Lys-Leu-NH2)-p-octiphenyl (1) and 14,84-bismethoxy-22,33,42,53,62,73-hexa(Gla-Leu-Lys-Leu-NH2)-p-octiphenyl (2) are described (Gla = -OCH2CO-). Nanomolar concns. of push-pull rod 1 are found to suffice to selectively form ion channels in polarized spherical bilayer membranes composed of egg yolk phosphatidylcholine. Exponential dependence of the ion-channel activity on membrane polarization reveals a gating charge of 0.85/channel. Independence of the activity of push-push rod 2 on membrane potential demonstrates that cell membrane recognition originates from the axial dipole in push-pull rod 1. Nonlinear concentration dependence of activity at -180 mV indicates parallel self-assembly of push-pull rod 1 into a tetrameric barrel-stave supramol.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

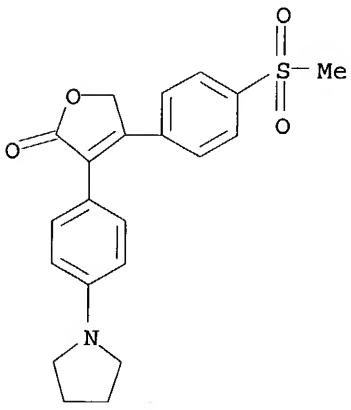
L3 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:816659 CAPLUS
DN 135:357924
TI Novel heterocyclic compounds, namely imidazole sulfones and analogs, with anti-inflammatory activity, their preparation, and their therapeutic use as cyclooxygenase 2 inhibitors
IN Almansa Rosales, Carmen; Gonzalez Gonzalez, Concepcion; Torres Barreda, M. Carmen
PA J. Uriach & Cia S.A., Spain
SO PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DT Patent
LA Spanish
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	WO 2001083475	A1	20011108	WO 2001-ES152		20010423
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
				ES 2000-1138	A	20000425
	ES 2166710	A1	20020416	ES 2000-1138		20000425
	BR 2001010328	A	20030107	BR 2001-10328		20010423
				ES 2000-1138	A	20000425
				WO 2001-ES152	W	20010423
	EP 1281709	A1	20030205	EP 2001-921386		20010423
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
				ES 2000-1138	A	20000425
				WO 2001-ES152	W	20010423
	JP 2003531903	T2	20031028	JP 2001-580903		20010423
				ES 2000-1138	A	20000425
				WO 2001-ES152	W	20010423
	NO 2002005101	A	20021220	NO 2002-5101		20021024
				ES 2000-1138	A	20000425
				WO 2001-ES152	W	20010423
	US 2003114456	A1	20030619	US 2002-258471		20021025
				ES 2000-1138	A	20000425
				WO 2001-ES152	W	20010423

OS MARPAT 135:357924
IT **372107-26-1P**, 4-Chloro-1-(4-methylsulfonylphenyl)-5-[4-(1-pyrrolidinyl)phenyl]imidazole **372107-51-2P**, 4-(4-Methylsulfonylphenyl)-3-[4-(1-pyrrolidinyl)phenyl]-5H-furan-2-one
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of imidazole sulfones and analogs as cyclooxygenase 2 inhibitors and antiinflammatories)
RN 372107-26-1 CAPLUS
CN 1H-Imidazole, 4-chloro-1-[4-(methylsulfonyl)phenyl]-5-[4-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



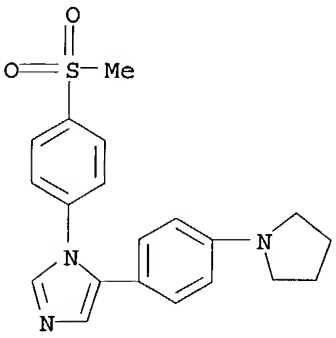
RN 372107-51-2 CAPLUS
CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-[4-(1-pyrrolidinyl)phenyl]-
(9CI) (CA INDEX NAME)



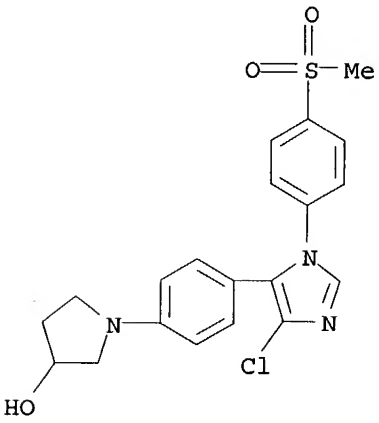
IT **372107-27-2P**, 1-(4-Methylsulfonylphenyl)-5-[4-(1-pyrrolidinyl)phenyl]imidazole **372107-28-3P**, 4-Chloro-5-[4-(3-hydroxypyrrolidin-1-yl)phenyl]-1-(4-methylsulfonylphenyl)imidazole **372107-29-4P**, 4-Chloro-5-[4-(2-methylpyrrolidin-1-yl)phenyl]-1-(4-methylsulfonylphenyl)imidazole **372107-31-8P**, 4-[4-Chloro-5-[4-(1-pyrrolidinyl)phenyl]imidazol-1-yl]benzenesulfonamide **372107-33-0P**, 4-Chloro-5-[3-chloro-4-(1-pyrrolidinyl)phenyl]-1-(4-methylsulfonylphenyl)imidazole **372107-35-2P**, 4-Chloro-1-(4-methylsulfonylphenyl)-5-[4-(2,5-dioxopyrrolidin-1-yl)phenyl]imidazole **372107-37-4P**, 4-Chloro-1-(4-methylsulfonylphenyl)-5-[4-(2-oxo-3-pyrrolin-1-yl)phenyl]imidazole **372107-39-6P**, 4-Chloro-1-(4-methylsulfonylphenyl)-5-[4-(2-oxooxazolidin-3-yl)phenyl]imidazole **372107-43-2P**, 4-Chloro-1-(4-methylsulfonylphenyl)-5-[4-(2-oxopyrrolidin-1-yl)phenyl]imidazole **372107-48-7P**, 3-[4-(2,5-Dioxopyrrolidin-1-yl)phenyl]-4-(4-methylsulfonylphenyl)-5H-furan-2-one **372107-49-8P**, 4-(4-Methylsulfonylphenyl)-3-[4-(2-oxo-3-pyrrolin-1-yl)phenyl]-5H-furan-2-one **372107-52-3P**, 3-[3-Chloro-4-(1-pyrrolidinyl)phenyl]-4-(4-methylsulfonylphenyl)-5H-furan-2-one **372107-54-5P**, 4-[5-[4-(2-Oxo-3-pyrrolin-1-yl)phenyl]-3-trifluoromethyl-1H-pyrazol-1-

yl]benzenesulfonamide **372107-55-6P**, 4-[5-[4-(1-Pyrrolidinyl)phenyl]-3-trifluoromethyl-1H-pyrazol-1-yl]benzenesulfonamide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of imidazole sulfones and analogs as cyclooxygenase 2 inhibitors and antiinflammatories)

RN 372107-27-2 CAPLUS
CN 1H-Imidazole, 1-[4-(methylsulfonyl)phenyl]-5-[4-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 372107-28-3 CAPLUS
CN 3-Pyrrolidinol, 1-[4-[4-chloro-1-[4-(methylsulfonyl)phenyl]-1H-imidazol-5-yl]phenyl]- (9CI) (CA INDEX NAME)



RN 372107-29-4 CAPLUS
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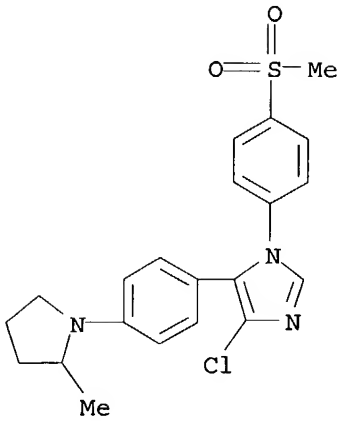
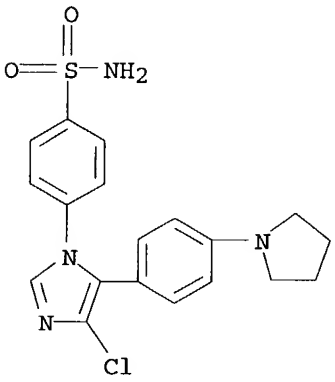
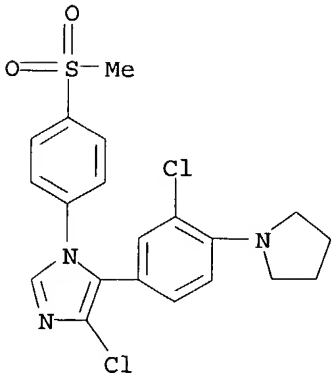


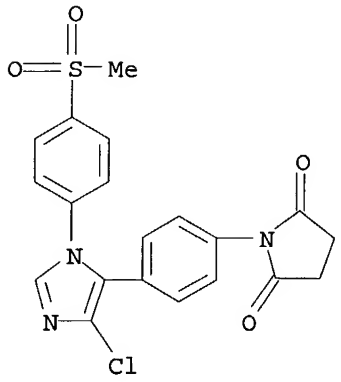
RN 372107-31-8 CAPLUS
CN Benzenesulfonamide, 4-[4-chloro-5-[4-(1-pyrrolidinyl)phenyl]-1H-imidazol-1-yl]- (9CI) (CA INDEX NAME)



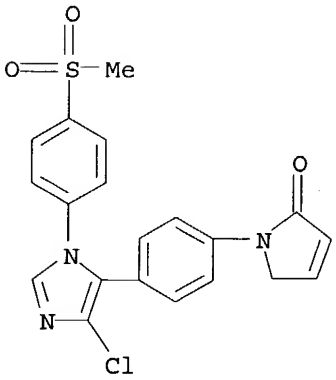
RN 372107-33-0 CAPLUS
CN 1H-Imidazole, 4-chloro-5-[3-chloro-4-(1-pyrrolidinyl)phenyl]-1-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RN 372107-35-2 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[4-[4-chloro-1-[4-(methylsulfonyl)phenyl]-1H-imidazol-5-yl]phenyl]- (9CI) (CA INDEX NAME)



RN 372107-37-4 CAPLUS
CN 2H-Pyrrol-2-one, 1-[4-[4-chloro-1-[4-(methylsulfonyl)phenyl]-1H-imidazol-5-yl]phenyl]-1,5-dihydro- (9CI) (CA INDEX NAME)



RN 372107-39-6 CAPLUS
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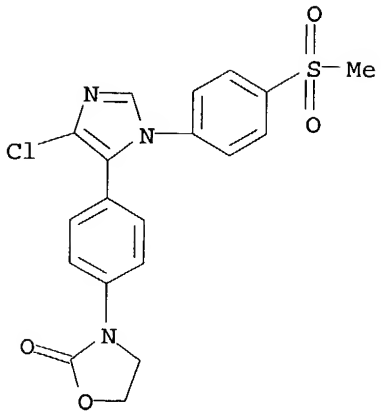

RN 372107-43-2 CAPLUS
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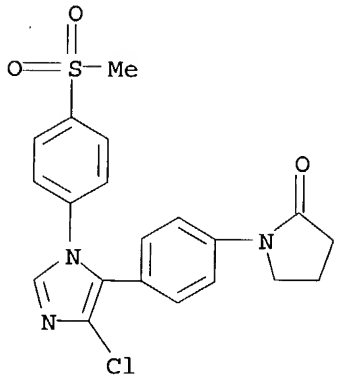

RN 372107-48-7 CAPLUS
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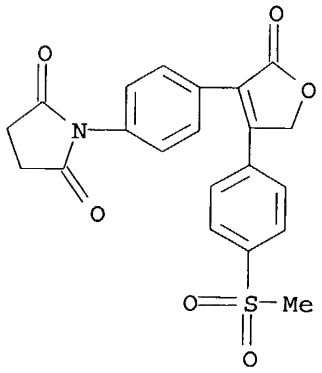
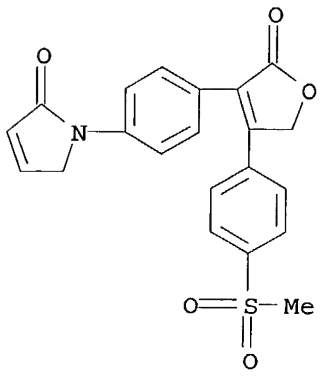
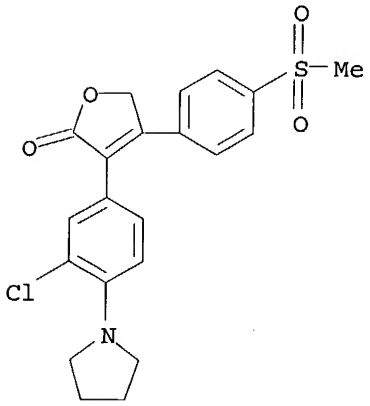


RN 372107-49-8 CAPLUS

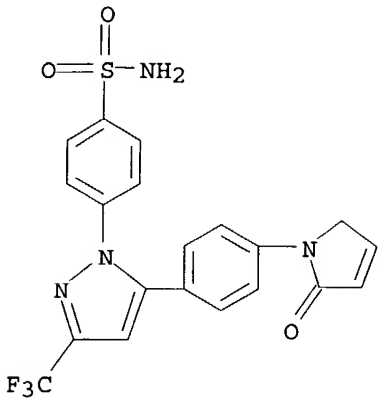
CN 2H-Pyrrol-2-one, 1-[4-[2,5-dihydro-4-[4-(methylsulfonyl)phenyl]-2-oxo-3-furanyl]phenyl]-1,5-dihydro- (9CI) (CA INDEX NAME)



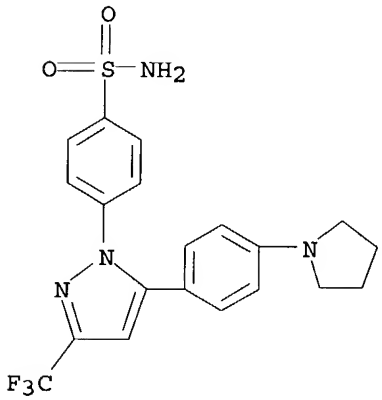
RN 372107-52-3 CAPLUS
CN 2(5H)-Furanone, 3-[3-chloro-4-(1-pyrrolidinyl)phenyl]-4-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RN 372107-54-5 CAPLUS
CN Benzenesulfonamide, 4-[5-[4-(2,5-dihydro-2-oxo-1H-pyrrol-1-yl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



RN 372107-55-6 CAPLUS
CN Benzenesulfonamide, 4-[5-[4-(1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



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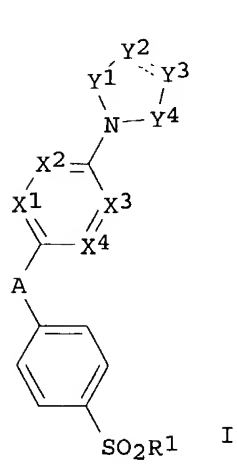

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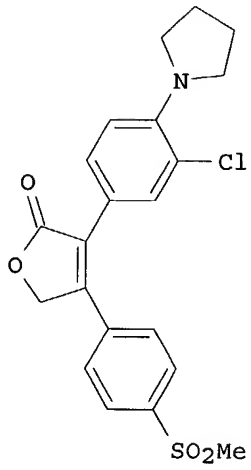


II

AB The invention relates to novel heterocyclic compds. of formula I, and to their salts, solvates, and prodrugs [wherein: A = 5-membered unsatd. or partially unsatd. ring with 1-3 optional heteroatoms (N/O/S), optional substituent(s) R2, and adjacent aryl groups; R1 = C1-8 (halo)alkyl, NR3R4; R2 = C1-4 (halo)alkyl, halo, oxo, cyano, NO2, CHO, COCH3, CO2R3; R3 = H, C1-8 alkyl, aryl, arylalkyl; R4 = H, C1-8 alkyl, arylalkyl, COR5, CO2R5; R5 = C1-8 (halo)alkyl; all X's = CR6; or 1-3 X's = N and the remainder = CR6; R6 = H, halo, C1-3 alkyl or alkoxy; dashed bond = optional pi bond; Y1, Y4 = CR7R7 or CO; Y2 and Y3 = CR8 when doubly bonded, or CR8R8 when singly bonded; Y2 can be CO if Y1 is not; Y3 can be CO if Y4 is not; Y3 can be NR9, O, or S if Y4 is CO; R7 = H, Me, Et; R8 = H, Me, Et, OH, OMe, or halo; R9 = H or C1-4 alkyl; aryl = Ph or naphthyl optionally substituted by C1-8 (halo)alkyl, halo, cyano, NO2, OR10, alkyl-OR10, SR10, alkyl-SR10, NR10R11, NR10COR11, COR10, CO2R10; R10 = H, C1-8 alkyl, CH2Ph, R11 = C1-8 (halo)alkyl]. The compds. are selective inhibitors of cyclooxygenase 2 (COX-2), useful as anti-inflammatory agents. Nineteen examples and 8 reference examples are given. For instance, 1-(4-methylsulfonylphenyl)ethanone underwent α-bromination, cyclocondensation with 4-nitrophenylacetic acid (60%), and hydrogenation at nitro (95%) to give 3-(4-aminophenyl)-4-(4-methylsulfonylphenyl)-5H-furan-2-one. This intermediate underwent cyclization with 1,4-dibromobutane at the amino group (27%) and adjacent ring chlorination (73%) to give title compound II. In tests for inhibition of COX-1 and COX-2 activity in human cell lines, II at 0.1 μM gave 93% inhibition of COX-2 but did not appreciably inhibit COX-1 (0%).

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:816651 CAPLUS
DN 135:358158
TI Preparation of N-[4-(oxadiazol-2-yl)phenylsulfonyl]-amino acid derivatives having therapeutic or preventive efficacies against glomerular disorders
IN Shinosaki, Toshihiro; Ninomiya, Mitsuyoshi; Watanabe, Fumihiko
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001083464	A1	20011108	WO 2001-JP3215	20010416
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
			JP 2000-120235	A 20000421

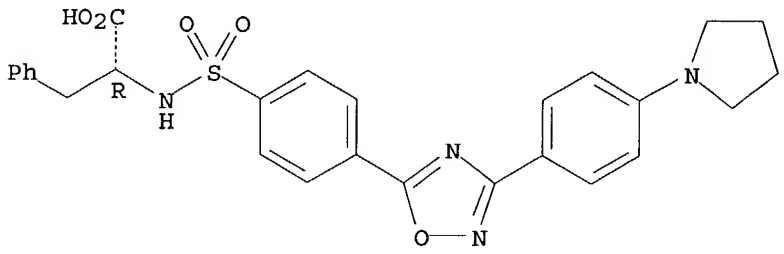
OS MARPAT 135:358158
IT **372106-16-6P**, (R)-2-[[[4-[3-(4-(Pyrrolidin-1-yl)phenyl)-1,2,4-oxadiazol-5-yl]phenyl]sulfonyl]amino]-2-benzylethanoic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [(oxadiazolyl)phenylsulfonyl]-amino acid derivs. as matrix metalloproteinase inhibitors and therapeutic or preventive agents for glomerular disorders)

RN 372106-16-6 CAPLUS

CN D-Phenylalanine, N-[[4-[3-[4-(1-pyrrolidinyl)phenyl]-1,2,4-oxadiazol-5-yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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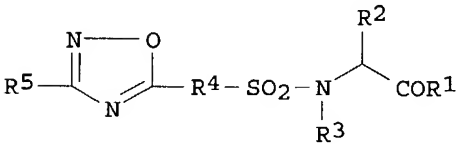


I

AB Pharmaceutical compns. for the treatment or prevention of glomerular disorders contain as the active ingredient compds. of the general formula [I; R1 = NHOH, OH, lower alkyloxy; R2, R3 = H, (un)substituted lower alkyl, aryl, aralkyl, heteroaryl, or heteroarylalkyl; R4 = (un)substituted arylene or heteroarylene; R5 = (un)substituted aryl, heteroaryl, or nonarom. heterocyclyl], prodrugs of the same, pharmaceutically acceptable salts of both, or solvates of them. These compds. I inhibit matrix metalloproteinase (MMP) and are safe and highly effective for the prevention or treatment of glomerular disorders, in particular glomerular nephritis and diabetic nephropathy. They are also useful for the treatment of osteoarthritis, aortic aneurysm, and diabetic retinopathy. Thus, N-sulfonylation of D-phenylalanine Me ester hydrochloride with 4-chlorosulfonylbenzoic acid in aqueous Na2CO3 at room temperature for 3 h gave N-(4-carboxyphenylsulfonyl)-L-phenylalanine Me ester which was converted into the acid chloride by treatment with oxalyl chloride in DMF at room temperature for 1 h and cyclocondensed with 4-fluorobenzamidoxime (preparation given) in pyridine and diglyme at room temperature for 1 h and then at 110° for 3 h, followed by saponification with a mixture of 1 N aqueous NaOH and DMSO and acidification with aqueous 2 N HCl to give N-[4-[3-(4-fluorophenyl)-1,2,4-oxadiazol-5-yl]phenylsulfonyl]-D-phenylalanine. N-[4-[3-(5-chlorothiophen-2-yl)-1,2,4-oxadiazol-5-yl]phenylsulfonyl]-L-valine showed IC50 of 0.0051, 0.056, and 0.025 μM against MMP-2, 8, and 9, resp.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

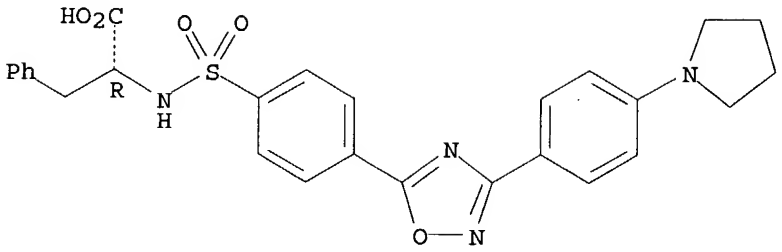
L3 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:816650 CAPLUS
DN 135:357931
TI Preparation of oxadiazole derivatives as anticancer agents inhibiting MMP-2
IN Yoshioka, Takayuki; Maekawa, Ryuji; Watanabe, Fumihiko
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001083463	A1	20011108	WO 2001-JP3214	20010416
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
				JP 2000-120234 A	20000421
	AU 2001046916	A5	20011112	AU 2001-46916	20010416
				JP 2000-120234 A	20000421
				WO 2001-JP3214 W	20010416
	EP 1277744	A1	20030122	EP 2001-919938	20010416
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
				JP 2000-120234 A	20000421
				WO 2001-JP3214 W	20010416
	BR 2001010211	A	20030603	BR 2001-10211	20010416
				JP 2000-120234 A	20000421
				WO 2001-JP3214 W	20010416
	ZA 2002008307	A	20031015	ZA 2002-8307	20021015
				JP 2000-120234 A	20000421
	NO 2002005035	A	20021219	NO 2002-5035	20021018
				JP 2000-120234 A	20000421
				WO 2001-JP3214 W	20010416
	US 2003203940	A1	20031030	US 2002-257917	20021018
	US 6720343	B2	20040413		
				JP 2000-120234 A	20000421
				WO 2001-JP3214 W	20010416
	US 2004122066	A1	20040624	US 2003-730946	20031210
				JP 2000-120234 A	20000421
				WO 2001-JP3214 W	20010416
				US 2002-257917 A3	20021018

OS MARPAT 135:357931
IT **372106-16-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oxadiazole derivs. as anticancer agents inhibiting MMP-2)
RN 372106-16-6 CAPLUS
CN D-Phenylalanine, N-[[4-[3-[4-(1-pyrrolidinyl)phenyl]-1,2,4-oxadiazol-5-yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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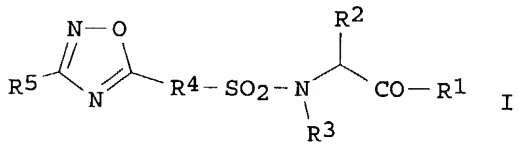

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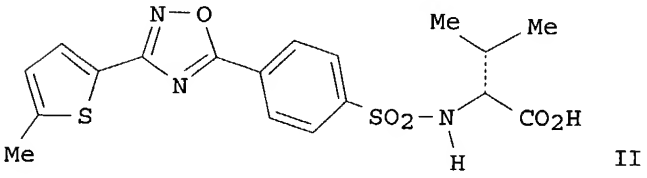


II

AB The title compds. I [R1 is hydroxyl or the like; R2 is optionally substituted lower alkyl or the like; R3 is hydrogen or the like; R4 is optionally substituted arylene or the like; and R5 is optionally substituted aryl or the like] are prepared The title compound II in vitro showed IC50 of 6 nM against MMP-2. Formulations are given.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:816648 CAPLUS
DN 135:344729
TI Preparation of N-thiazolylphenylsulfonylamino acid and N-oxazolylphenylsulfonylamino acid derivatives as macrophage metalloelastase inhibitors
IN Furue, Shingo; Watanabe, Fumihiko; Tamura, Yoshinori
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001083461	A1	20011108	WO 2001-JP3437	20010423

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,

HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

JP 2000-130041	A	20000428
JP 2000-293419	A	20000927

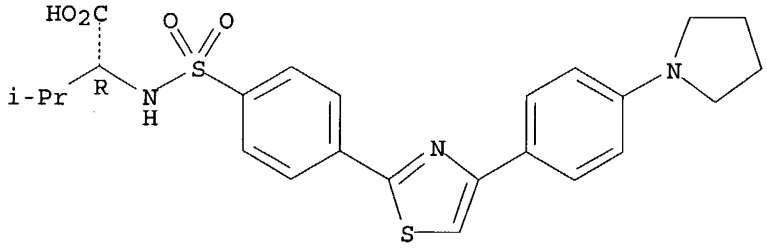
OS MARPAT 135:344729

IT **370597-61-8P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-thiazolylphenylsulfonylamino acid and N-oxazolylphenylsulfonylamino acid derivs. as macrophage metalloelastase inhibitors)

RN 370597-61-8 CAPLUS

CN D-Valine, N-[[4-[4-[4-(1-pyrrolidinyl)phenyl]-2-thiazolyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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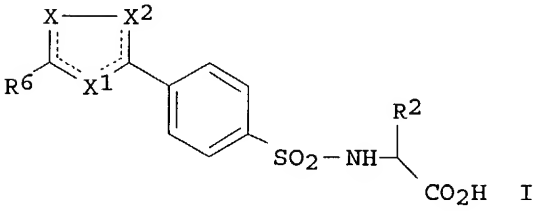

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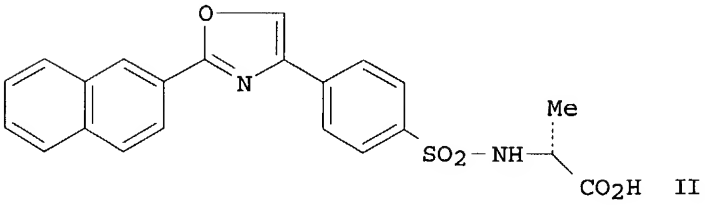


II

AB Title compds. [I; X = O, N, S, CH; X1 = N, O; X2 = CH, S; dotted bond = single bond, double bond; R6 = (un)substituted aryl, benzofuranyl, benzothienyl; R2 = alkyl], optical isomers, prodrugs, and pharmaceutically

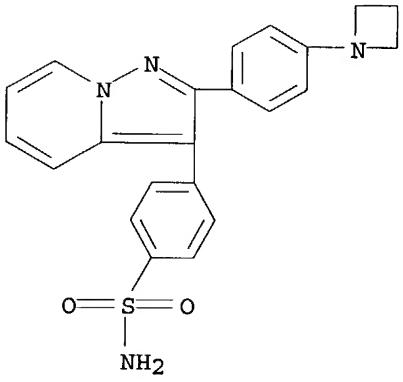
acceptable salts or solvates of title compds. are prepared as macrophage metalloelastase inhibitors. Thus, the title compound II was prepared and MMP-1, MMP-2, MMP-8, MMP-9, MMP-12, and MMP-13 inhibition tested.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:371567 CAPLUS
DN 135:5612
TI Preparation of new pyrazolo terpyridines as remedies for inflammation, autoimmune diseases
IN Yamamoto, Hirofumi; Takahashi, Fumie; Kato, Takeshi; Nakamura, Katsuya; Manabe, Koji
PA Fujisawa Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 64 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001139575	A2	20010522	JP 1999-323692	19991115
			JP 1999-323692	19991115

OS MARPAT 135:5612
IT **340322-50-1P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of new pyrazolo terpyridines as remedies for inflammation autoimmune diseases)
RN 340322-50-1 CAPLUS
CN Benzenesulfonamide, 4-[2-[4-(1-azetidinyl)phenyl]pyrazolo[1,5-a]pyridin-3-yl]- (9CI) (CA INDEX NAME)



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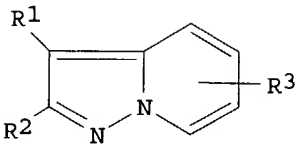

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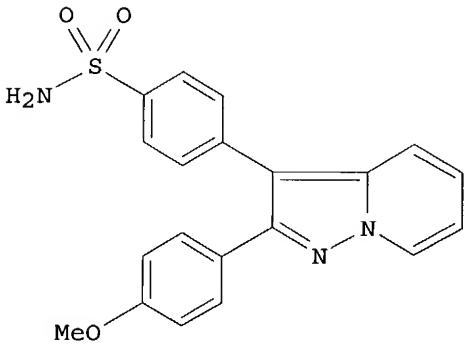


II

AB The pyrazolo terpyridine or that salt which is cyclooxygenase - 2 (COX-II) inhibitors, those production methods, the medicine composition, and the person or the animal which contain those inflammation condition, u painfully, prevention of the autoimmune disease and / or the method of treating is offered. Below-mentioned general formula (I) [in the formula, the R1 and the R2, the resp. hydrogen, the hydrogen, the low-grade alkyl group and the halogen et cetera, mean, R3 such as low-grade alkyl group and the cyclo (low grade) alkyl group resp.] So the chemical compound which is displayed or that salt.

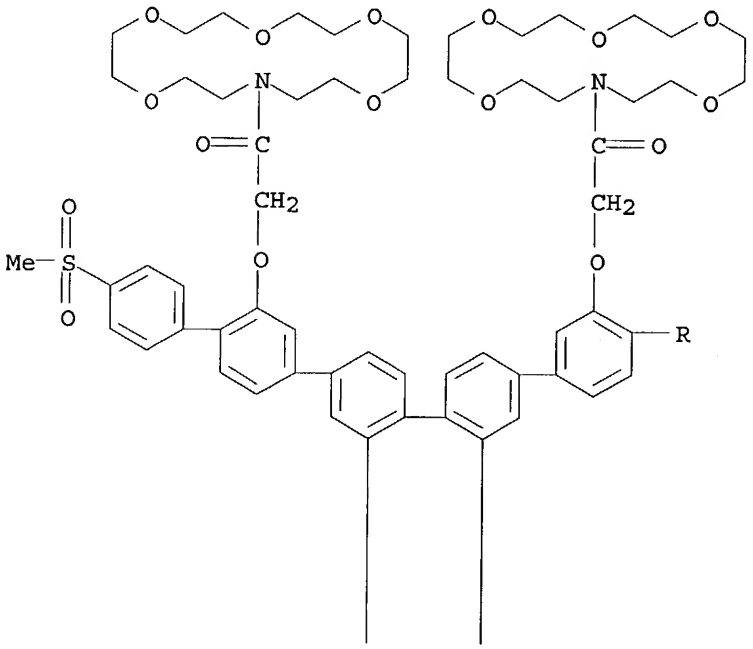
L3 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:130219 CAPLUS
DN 134:322321
TI Electrostatics of Cell Membrane Recognition: Structure and Activity of Neutral and Cationic Rigid Push-Pull Rods in Isoelectric, Anionic, and Polarized Lipid Bilayer Membranes
AU Sakai, Naomi; Gerard, David; Matile, Stefan
CS Department of Organic Chemistry, University of Geneva, Geneva, CH-1211, Switz.
SO Journal of the American Chemical Society (2001), 123(11), 2517-2524
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 134:322321
IT **335629-09-9P 335629-19-1P 335629-21-5P**
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(electrostatics of cell membrane recognition: structure and activity of neutral and cationic rigid push-pull rods in isoelec., anionic, and polarized lipid bilayer membranes)

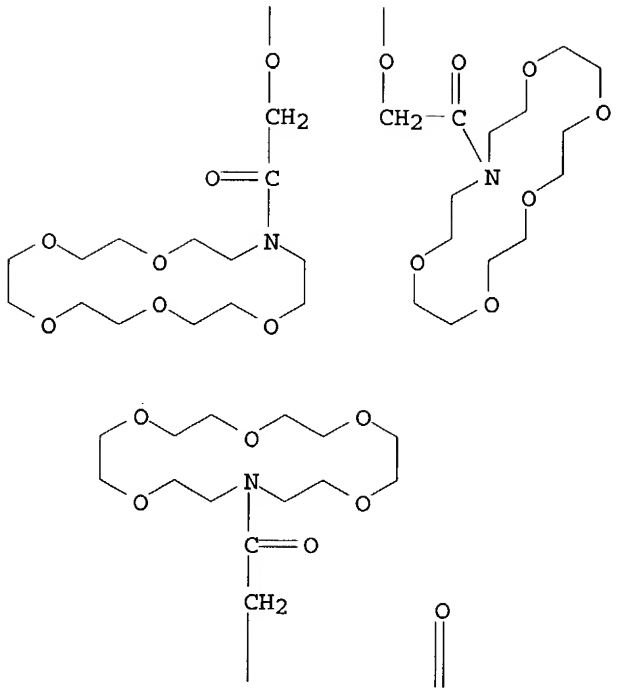
RN 335629-09-9 CAPLUS

CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16,16',16'',16''',16'''',16'''''-[[4,4''''''-bis(methylsulfonyl)[1,1':4',1'':4'',1''':4''',1'''':4'''',1'''''':4'''''',1''''''':4''''''',1'''''''-octiphenyl]-2',2''',2'''''',3'',3'''',3''''''-hexayl]hexakis[oxy(1-oxo-2,1-ethanediyl)]]hexakis- (9CI) (CA INDEX NAME)

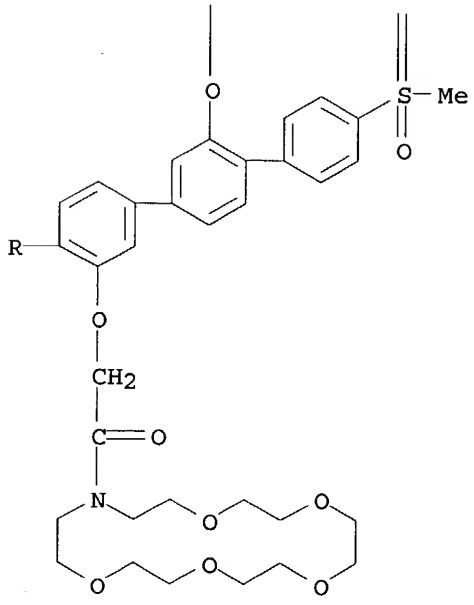
PAGE 1-A



PAGE 2-A



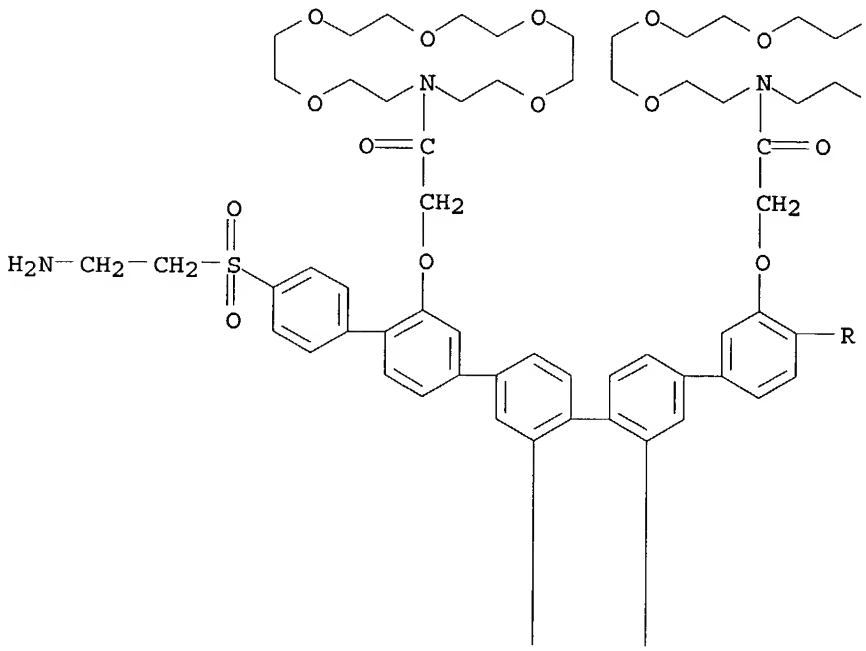
PAGE 3-A



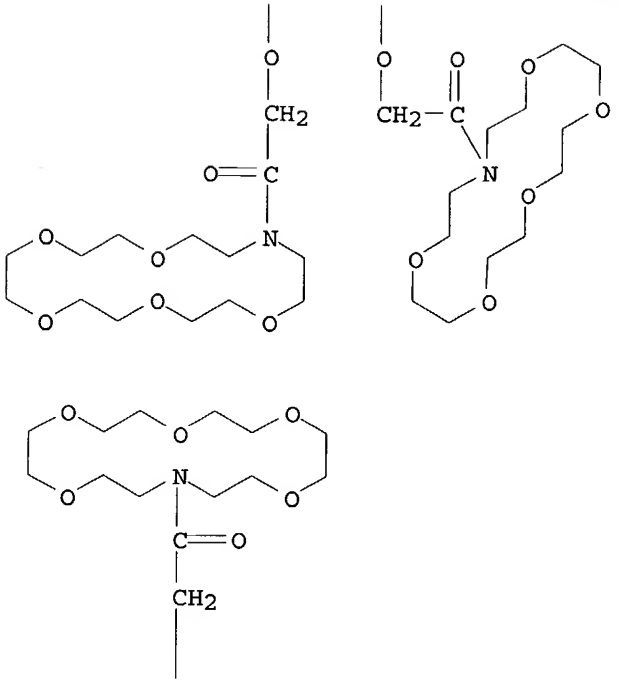
RN 335629-19-1 CAPLUS
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16,16',16'',16''',16'''',16'''''-[[4-[(2-aminoethyl)sulfonyl]-4''''''-(methylthio)[1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1'''''':4'''''',1''''''':4''''''',1'''''''-octiphenyl]-

2',2''',2''''',3'',3'''',3''''''-hexayl]hexakis[oxy(1-oxo-2,1-ethanediyl)]]hexakis- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



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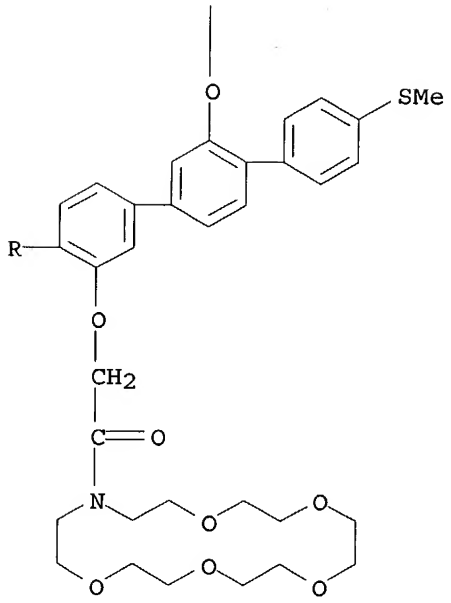
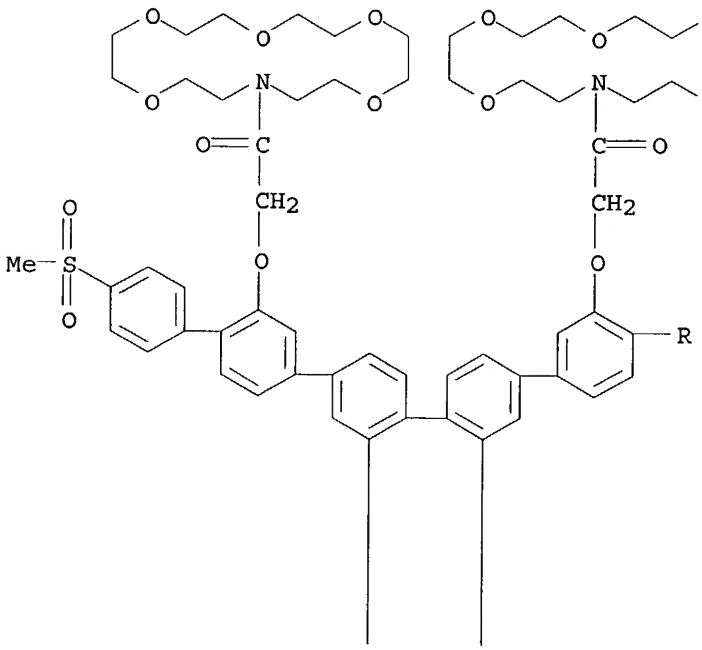


RN 335629-21-5 CAPLUS
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16,16',16'',16''',16'''',16'''''-[[4-[(2-aminoethyl)thio]-4'''''''-(methylsulfonyl)[1,1':4',1'':4'',1'''':4''',1'''':4'''',1''''':4''''',1'''''':4'''''',1''''''':4'''''''-octiphenyl]-

2',2''',2''''',3'',3'''',3''''''-hexayl]hexakis[oxy(1-oxo-2,1-ethanediyl)]]hexakis- (9CI) (CA INDEX NAME)

PAGE 1-A



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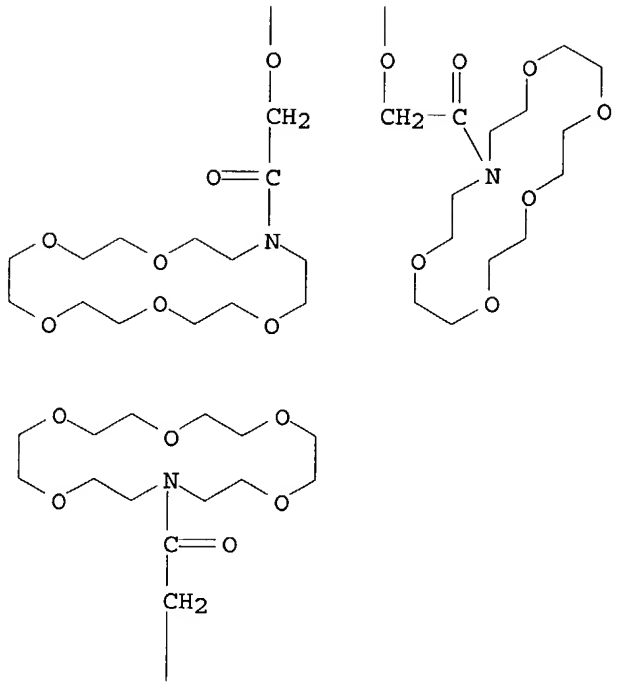

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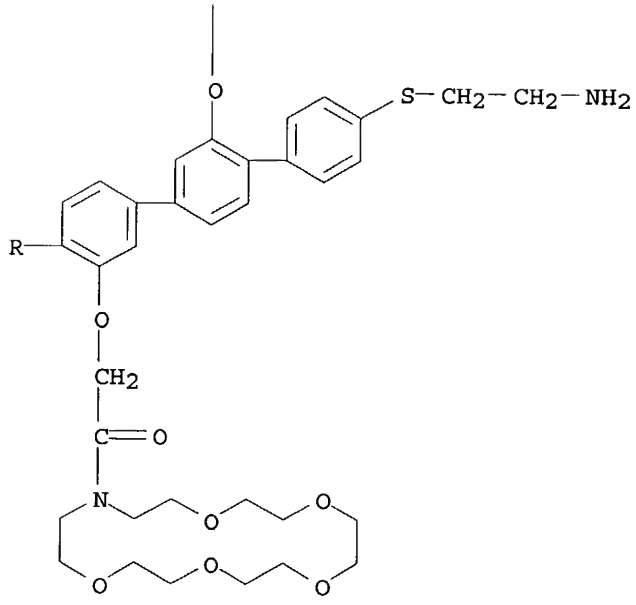


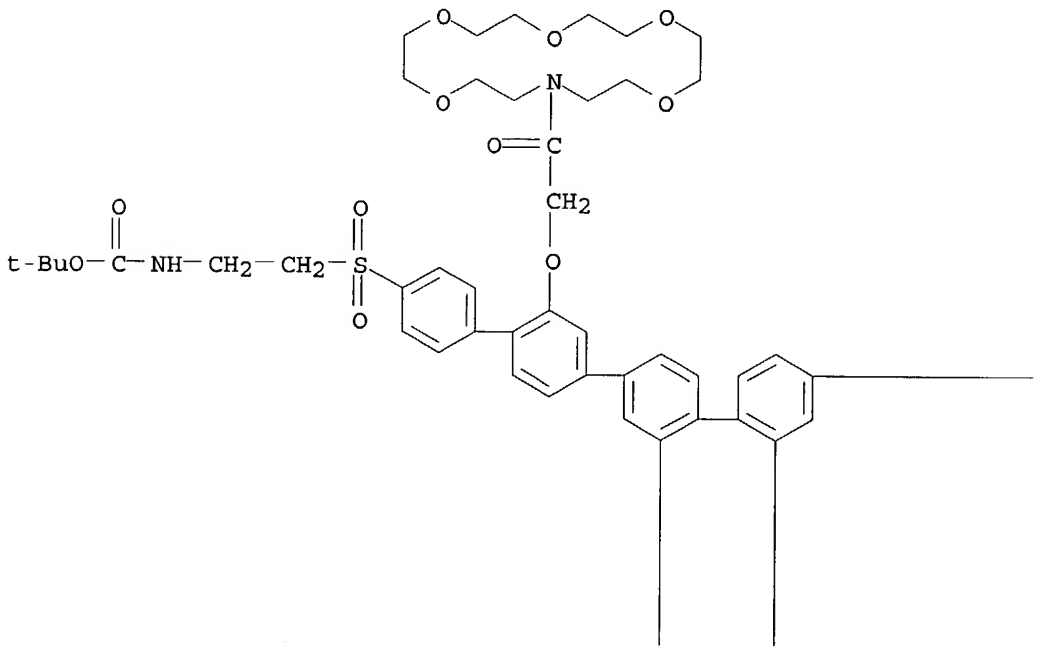
IT **335629-11-3P 335629-13-5P 335629-15-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(electrostatics of cell membrane recognition: structure and activity of

neutral and cationic rigid push-pull rods in isoelec., anionic, and polarized lipid bilayer membranes)

RN 335629-11-3 CAPLUS

CN Carbamic acid, [2-[[4'''''''-(methylsulfonyl)-2',2''',2''''',3'',3'''',3''''''-hexakis[2-oxo-2-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-yl)ethoxy][1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1''''''':4''''''',1'''''''-octiphenyl]-4-yl]sulfonyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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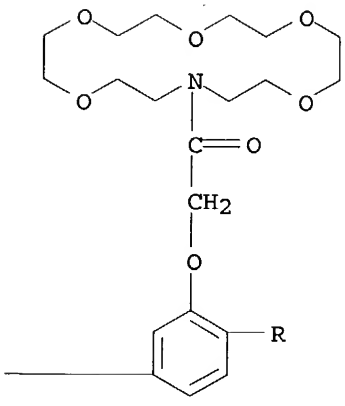

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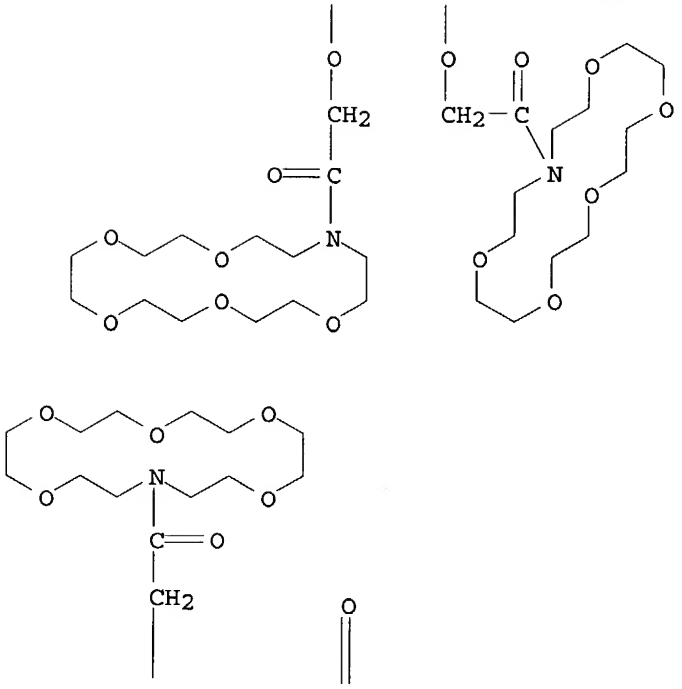

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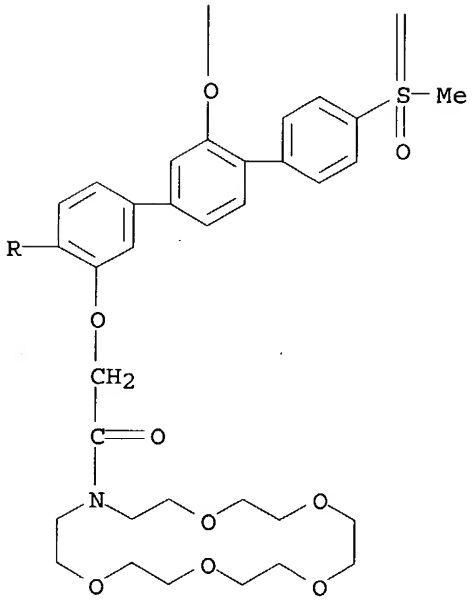
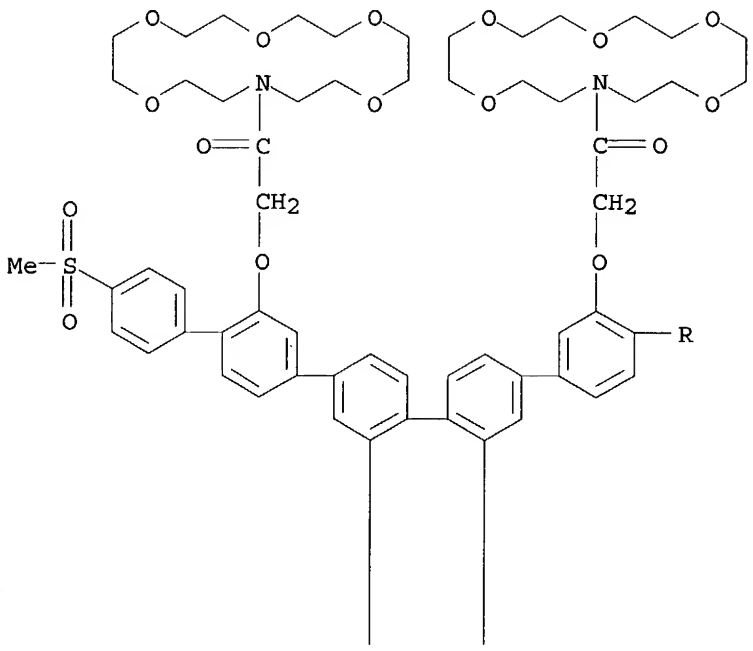


RN 335629-13-5 CAPLUS
CN Carbamic acid, [2-[[4'''''''-(methylsulfonyl)-2',2''',2''''',3'',3'''',3''''''-hexakis[2-oxo-2-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-yl)ethoxy][1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1'''''':4'''''',1''''''':4''''''',1'''''''-octiphenyl]-4-yl]thio]ethyl]-,

1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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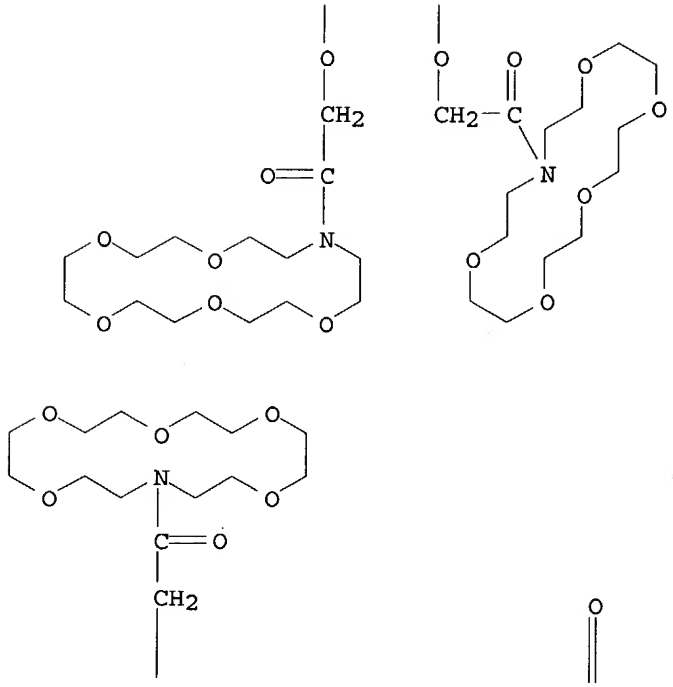
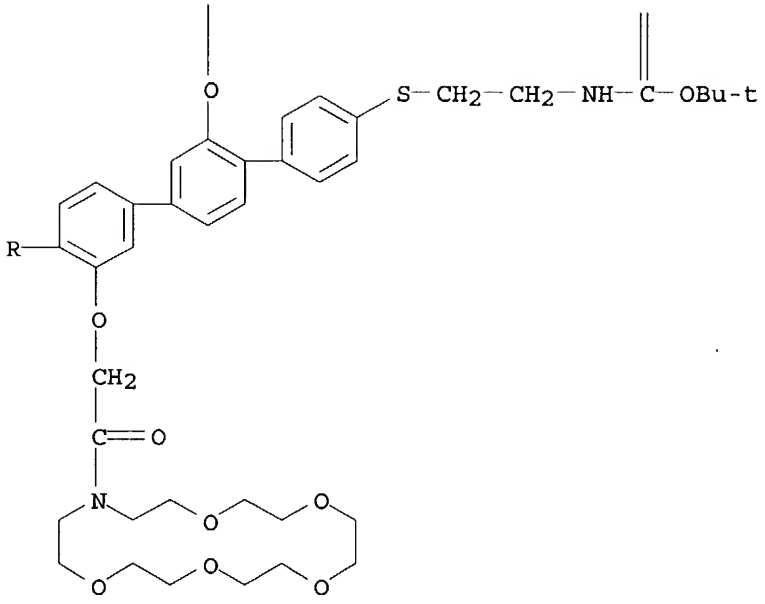
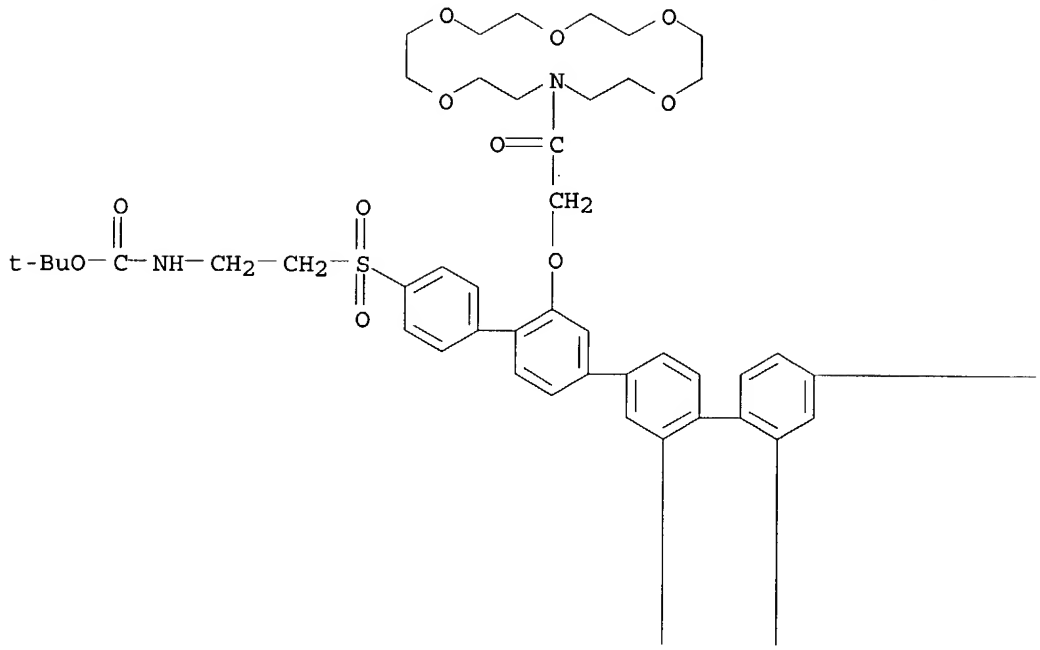




RN 335629-15-7 CAPLUS
CN Carbamic acid, [2-[[4''''''''-(methylthio)-2',2''',2''''',3'',3'''',3''''''-hexakis[2-oxo-2-(1,4,7,10,13-pentaoxa-16-azacyclooctadec-16-yl)ethoxy][1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1'''''':4''''',1''''''':4''''',1''''''''-octiphenyl]-4-yl]sulfonyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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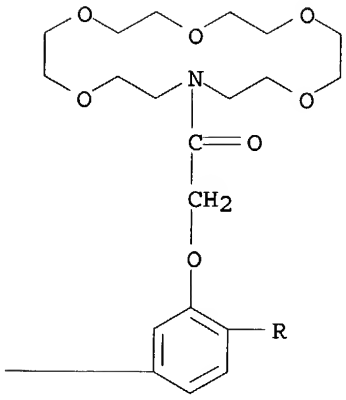

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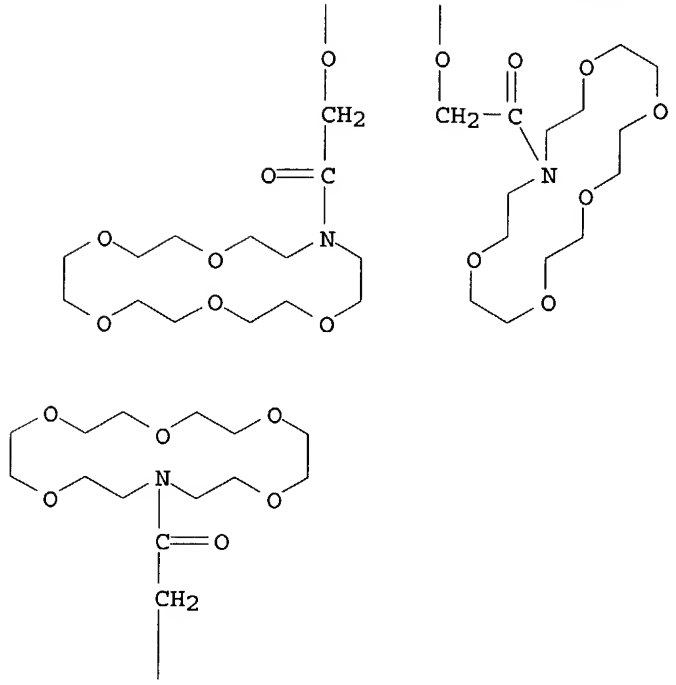

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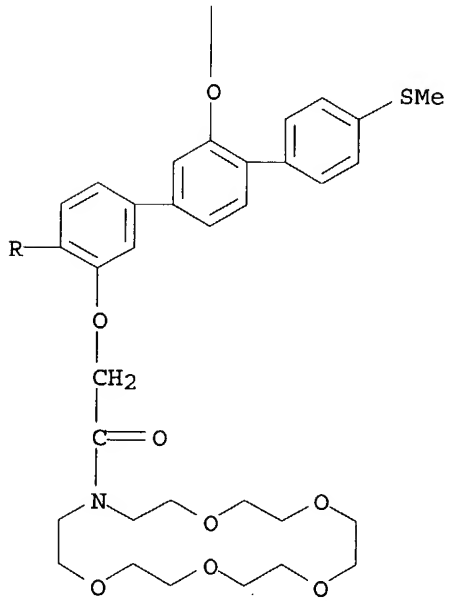
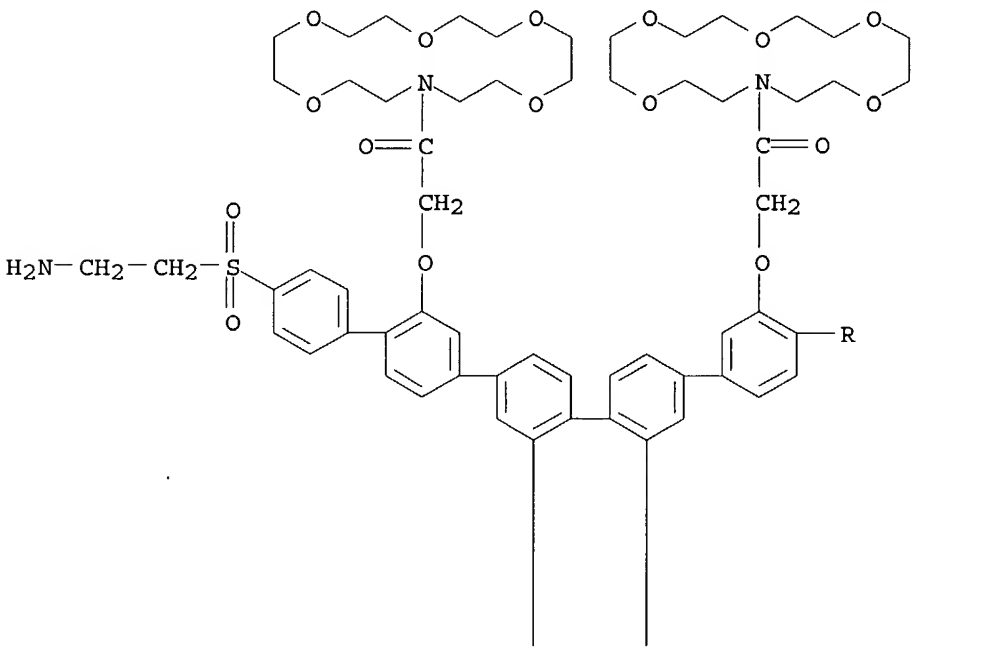


IT **335629-23-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(electrostatics of cell membrane recognition: structure and activity of neutral and cationic rigid push-pull rods in isoelec., anionic, and polarized lipid bilayer membranes)

RN 335629-23-7 CAPLUS
CN 1,4,7,10,13-Pentaoxa-16-azacyclooctadecane, 16,16',16'',16''',16'''',16'''''-[[4-[(2-aminoethyl)sulfonyl]-4'''''''-(methylsulfonyl)[1,1':4',1'':4'',1''':4''',1'''':4'''',1''''':4''''',1'''''':4'''''',1''''''':4'''''''-octiphenyl]-2',2''',2''''',3'',3'''',3''''''-hexayl]hexakis[oxy(1-oxo-2,1-ethanediyl)]]hexakis- (9CI) (CA INDEX NAME)

PAGE 1-A



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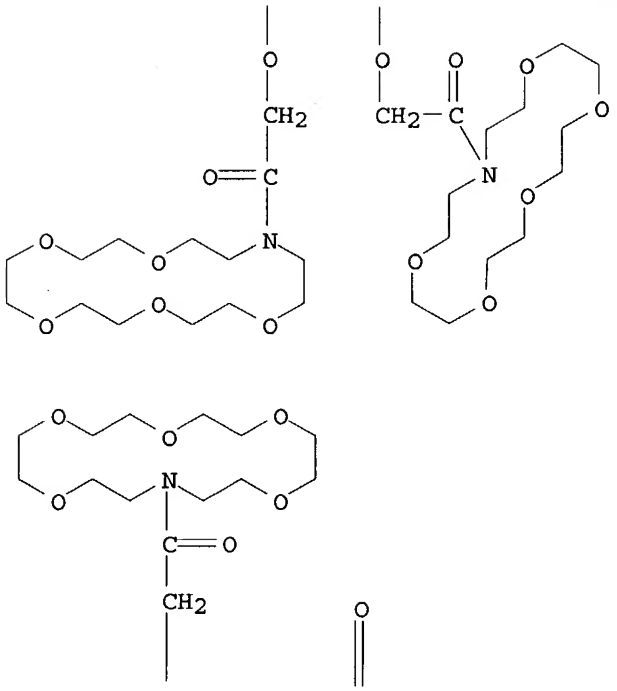

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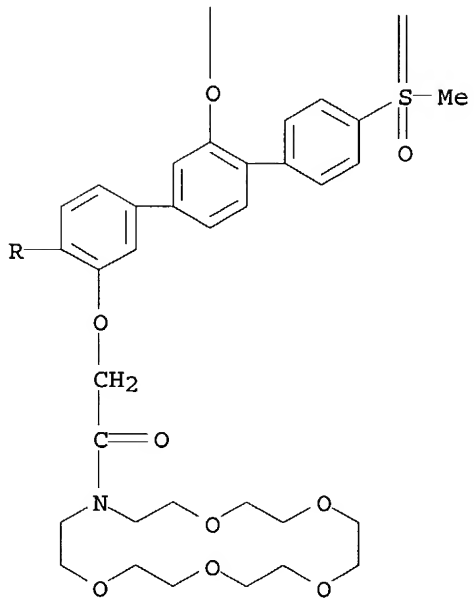


AB Design, synthesis, and structural and functional studies of rigid-rod ionophores of different axial electrostatic asymmetry are reported. The employed design strategy emphasized presence of (a) a rigid scaffold to minimize the conformational complexity, (b) a unimol. ion-conducting

pathway to minimize the suprastructural complexity and monitor the function, (c) an extended fluorophore to monitor structure, (d) variable axial rod dipole, and (e) variable terminal charges to create axial asymmetry. Studies in isoelec., anionic, and polarized bilayer membranes confirmed a general increase in activity of uncharged rigid push-pull rods in polarized bilayers. The similarly increased activity of cationic rigid push-pull rods with an electrostatic asymmetry comparable to that of α-helical bee toxin melittin (pos. charge near neg. axial dipole terminus) is shown by fluorescence-depth quenching expts. to originate from the stabilization of transmembrane rod orientation by the membrane potential. The reduced activity of rigid push-pull rods having an electrostatic asymmetry comparable to that in α-helical natural antibiotics (a pos. charge near the pos. axial dipole terminus) is shown by structural studies to originate from rod "ejection" by membrane potentials comparable to that found in mammalian plasma membranes. This structural evidence for cell membrane recognition by asym. rods is unprecedented and of possible practical importance with regard to antibiotic resistance.

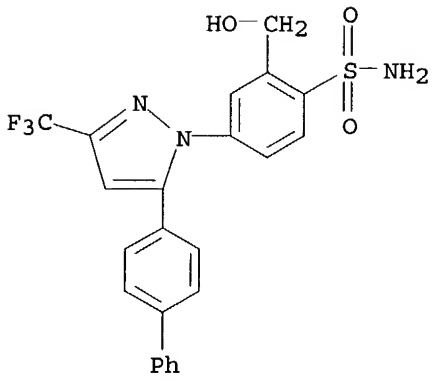
RE.CNT 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:790480 CAPLUS
DN 133:335232
TI Preparation of pyrazoles as antiinflammatory agents
IN Lohray, Vidya Bhushan; Sunil, Kumar Singh; Akella, Venkateswarlu; Lohray, Braj Bhushan; Pamulapati, Ganapathi Reddy; Ramanujam, Rajagopalan; Parimal, Misra
PA Reddy's Research Foundation, India
SO PCT Int. Appl., 134 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000066562	A1	20001109	WO 2000-IB556	20000502

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
IN 1999-MA508 A 19990503

OS MARPAT 133:335232
IT **304648-26-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazoles as antiinflammatory agents)
RN 304648-26-8 CAPLUS
CN Benzenesulfonamide, 4-[5-[1,1'-biphenyl]-4-yl-3-(trifluoromethyl)-1H-pyrazol-1-yl]-2-(hydroxymethyl)- (9CI) (CA INDEX NAME)



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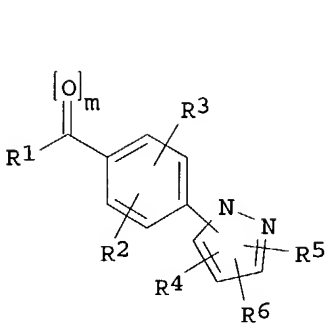
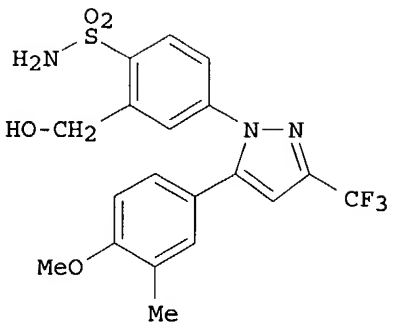


I



II

AB The title compds. [I; R1 = NH2, alkyl, alkylamino, etc.; R2 = CN, NO2, N3, etc.; R3 = H, halo, OH, etc.; R4-R6 = H, halo, OH, etc.; m = 0-2], useful for the treatment and/or prophylaxis of diseases of cyclooxygenase, more particularly COX-2, were prepared E.g., a multi-step synthesis of the pyrazole II which showed IC50 of 0.56 ± 0.03 (100 μM) against COX-2 vs. IC50 of 264 ± 0.5 (100 μM) against COX-1, was given.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:756693 CAPLUS
DN 133:309896
TI Preparation of sulfonamide derivatives having oxadiazole rings as matrix metalloprotease inhibitors
IN Watanabe, Fumihiko; Tamura, Yoshinori; Fujii, Yasuhiko
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI WO 2000063194 A1 20001026 WO 2000-JP2404 20000413
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
JP 1999-110321 A 19990419

EP 1172361 A1 20020116 EP 2000-915504 20000413
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
JP 1999-110321 A 19990419
WO 2000-JP2404 W 20000413

AU 765203 B2 20030911 AU 2000-36776 20000413
JP 1999-110321 A 19990419
WO 2000-JP2404 W 20000413

US 6495578 B1 20021217 US 2001-959008 20011017
JP 1999-110321 A 19990419
WO 2000-JP2404 W 20000413

NO 2001005078 A 20011218 NO 2001-5078 20011018
JP 1999-110321 A 19990419
WO 2000-JP2404 W 20000413

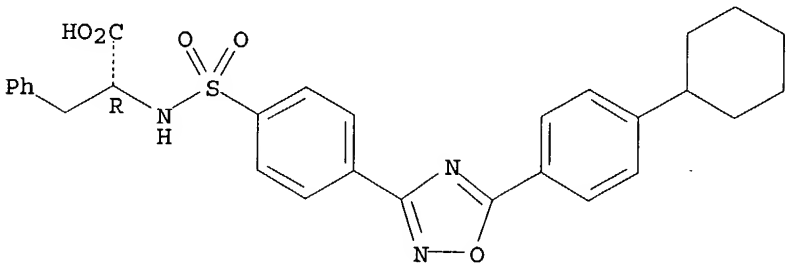
OS MARPAT 133:309896

IT **301835-77-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of sulfonamide derivs. having oxadiazole rings as matrix metalloprotease inhibitors)

RN 301835-77-8 CAPLUS

CN D-Phenylalanine, N-[[4-[5-(4-cyclohexylphenyl)-1,2,4-oxadiazol-3-yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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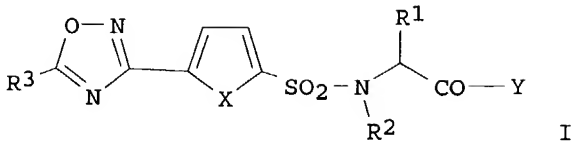

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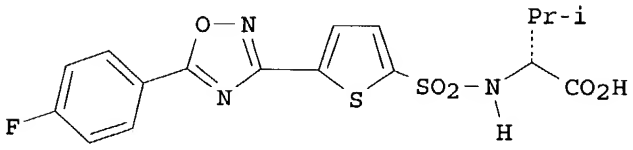

II

AB The title compds. I [R1 and R2 are each independently hydrogen, optionally substituted lower alkyl, or the like; R3 is optionally substituted aryl, optionally substituted heteroaryl, or the like; X is CH:CH, O, or S; and Y is NHOH, hydroxyl, or lower alkyloxy] are prepared The title compound II in vitro showed IC50 of 0.067 μM against MMP-2. Formulations are given.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:742084 CAPLUS
DN 133:309836
TI Preparation of 4,5-diaryl-3(2H)-furanones as cyclooxygenase-2 inhibitors
IN Shin, Song Seok; Noh, Min-Soo; Byun, Young Joo; Choi, Jin Kyu; Kim, Jin Kwan; Lim, Kyung Min; Kim, Ji Young; Choi, Young Hoon; Ha, Jun-Yong; Lee, Ki-Wha; Moh, Joo Hyun; Jeong, Yeon Su; Chung, Shin; Joo, Yung Hyup; Lee, Chang Hoon; Kang, Seon Hwa; Park, Young-Ho; Yi, Jung Bum
PA Pacific Corporation, S. Korea
SO PCT Int. Appl., 240 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000061571	A1	20001019	WO 2000-KR339	20000412
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
			KR 1999-13170	A 19990414
			KR 1999-29779	A 19990722
			KR 1999-39043	A 19990913
			KR 2000-16866	A 20000331
			KR 2000-17647	A 20000404
KR 2000066223	A	20001115	KR 1999-13170	19990414
KR 2001010728	A	20010215	KR 1999-29779	19990722
EP 1109799	A1	20010627	EP 2000-921133	20000412
EP 1109799	B1	20031217		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO

			KR 1999-13170	A	19990414
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			KR 2000-16866	A	20000331
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			WO 2000-KR339	W	20000412
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			KR 1999-13170	A	19990414
			KR 1999-29779	A	19990722
			KR 1999-39043	A	19990913
			KR 2000-16866	A	20000331
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			KR 1999-39043	A	19990913
			KR 2000-16866	A	20000331
			KR 2000-17647	A	20000404
			WO 2000-KR339	W	20000412
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			KR 2000-16866	A	20000331
			KR 2000-17647	A	20000404
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			KR 1999-29779	A	19990722
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			KR 1999-13170	A	19990414
			KR 1999-29779	A	19990722
			KR 1999-39043	A	19990913
			KR 2000-16866	A	20000331
			KR 2000-17647	A	20000404
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			KR 1999-13170	A	19990414
			KR 1999-29779	A	19990722
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			KR 2000-17647	A	20000404
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ZA 2001008089	A	20030102	ZA 2001-8089		20011002
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NO 2001004986	A	20011101	NO 2001-4986		20011012
			KR 1999-13170	A	19990414
			KR 1999-29779	A	19990722
			KR 1999-39043	A	19990913
			KR 2000-16866	A	20000331
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			WO 2000-KR339	W	20000412
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			KR 1999-13170	A	19990414
			KR 1999-29779	A	19990722

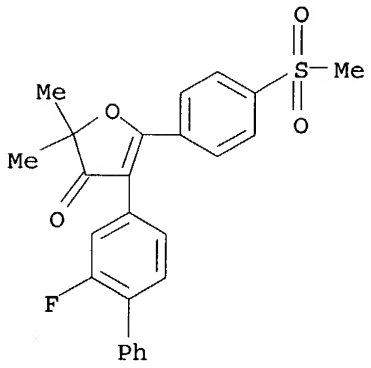
KR 1999-39043	A	19990913
KR 2000-16866	A	20000331
KR 2000-17647	A	20000404
WO 2000-KR339	W	20000412

OS MARPAT 133:309836

IT **301690-35-7P 301691-71-4P 301693-02-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4,5-diaryl-3(2H)-furanones as cyclooxygenase-2 inhibitors)

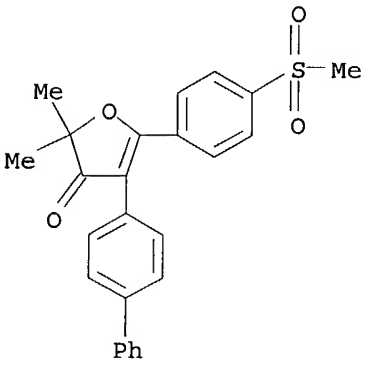
RN 301690-35-7 CAPLUS

CN 3(2H)-Furanone, 4-(2-fluoro[1,1'-biphenyl]-4-yl)-2,2-dimethyl-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



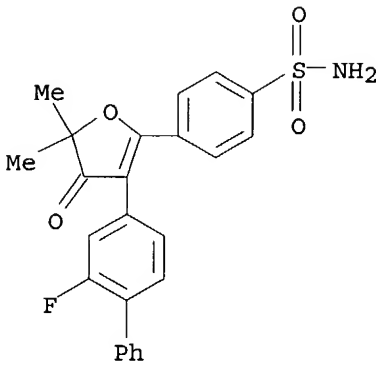
RN 301691-71-4 CAPLUS

CN 3(2H)-Furanone, 4-[1,1'-biphenyl]-4-yl-2,2-dimethyl-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

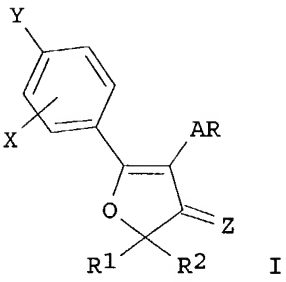


RN 301693-02-7 CAPLUS

CN Benzenesulfonamide, 4-[3-(2-fluoro[1,1'-biphenyl]-4-yl)-4,5-dihydro-5,5-dimethyl-4-oxo-2-furanyl]- (9CI) (CA INDEX NAME)



GI



I

AB The title compds. [I; X = halo, H, alkyl; Y = alkylsulfonyl, aminosulfonyl, alkylsulfinyl, etc.; Z = O, S; R1, R2 = alkyl; R1 and R2, taken together with the 2-position carbon atom of 3(2H)-furanone ring, form a 4-6 membered aliphatic or heterocyclic ring; AR = (un)substituted aryl of 5-10 atoms] which inhibit strongly and selectively COX-2 over COX-1 (data given), and are useful in treating inflammation, inflammation-associated disorders, and COX-2 mediated diseases, were prepared Thus, reacting 4-bromo-2,2-dimethyl-5-{4-(methylsulfonyl)phenyl}-3(2H)-furanone (preparation given) with 3-fluorobenzeneboronic acid in the presence of Pd(PPh3)4 and saturated aqueous NaHCO3 in PhMe and EtOH afforded I [X = H; Y = SO2Me; Z = O; R1, R2 = Me; AR = 3-FC6H4] which showed IC50 of 0.02 μg/mL against COX-2 vs. IC50 of 5 μg/mL against COX-1.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l3 and prostagladin
L4 0 L3 AND PROSTAGLADIN

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	92.70	248.33

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL